JUNE 1997

ISSN 0009-2614

CHEMICAL PHYSICS LETTERS

Editors: **DAVID BUCKINGHAM**

DAVID KING

AHMED ZEWAIL

MASTER INDEX VOLUMES 261–270
OCTOBER 1996 – MAY 1997

NORTH-HOLLAND

EDITORS: A.D. BUCKINGHAM, D.A. KING, A.H, ZEWAIL
Assistant Editor: Dr. R. Kobayashi, Cambridge, UK

FOUNDING EDITORS: G.J. HOYTINK, L. JANSEN
FORMER EDITORS: R.B. BERNSTEIN, D.A. SHIRLEY, R.N. ZARE

ADVISORY EDITORIAL BOARD

Australia
B.J. ORR, Sydney

Canada
P.A. HACKETT, Ottawa
J.W. HEPBURN, Waterloo
C.A. McDOWELL, Vancouver

Czech Republic
Z. HERMAN, Prague

Denmark
F. BESENBACHER, Aarhus
G.D. BILLING, Copenhagen

France
E. CLEMENTI, Strasbourg
J. DURUP, Toulouse
J.-M. LEHN, Strasbourg
J.-L. MARTIN, Palaiseau
B. SOEP, Orsay

Germany
R. AHLRICHS, Karlsruhe
V.E. BONDYBEY, Garching
W. DOMCKE, Dusseldorf
G. ERTL, Berlin
G. GERBER, Würzburg
G.L. HOFACKER, Garching
D.M. KOLB, Ulm
J. MANZ, Berlin
M. PARRINELLO, Stuttgart
S.D. PEYERIMHOFF, Bonn
R. SCHINKE, Göttingen
E.W. SCHLAG, Garching
J. TROE, Göttingen
H.C. WOLF, Stuttgart
W. ZINTH, Munich

India
C.N.R. RAO, Bangalore

Israel
J. JORTNER, Tel Aviv
R.D. LEVINE, Jerusalem

Italy
V. AQUILANTI, Perugia

Japan
H. HAMAGUCHI, Tokyo
M. ITO, Okazaki
T. KOBAYASHI, Tokyo
K. KUCHITSU, Sakado
H. NAKATSUJI, Kyoto
K. TANAKA, Tokyo
K. YOSHIHARA, Ishikawa

People's Republic of China
C.-H. ZHANG, Beijing

Poland
Z.R. GRABOWSKI, Warsaw

Russian Federation
A.L. BUCHACHENKO, Moscow
V.S. LETOKHOV, Troitzk
Yu.N. MOLIN, Novosibirsk

Spain
A. GONZÁLEZ UREÑA, Madrid

Sweden
P.E.M. SIEGBAHN, Stockholm
V. SUNDSTRÖM, Lund

Switzerland
M. CHERGUI, Lausanne-Dorigny
R.R. ERNST, Zurich
M. QUACK, Zurich

Taiwan, ROC
Y.T. LEE, Taipei

The Netherlands
A.J. HOFF, Leiden
A.W. KLEYN, Amsterdam
D.A. WIERSMA, Groningen

United Kingdom
M.N.R. ASHFOLD, Bristol
G.S. BEDDARD, Leeds
M.S. CHILD, Oxford
D.C. CLARY, London
R. FREEMAN, Cambridge
R.H. FRIEND, Cambridge
N.C. HANDY, Cambridge
A.C. LEGON, Exeter
R.M. LYNDEN-BELL, Belfast
J.P. SIMONS, Oxford
I.W.M. SMITH, Birmingham

USA
P. AVOURIS, Yorktown Heights, NY
A.J. BARD, Austin, TX
A.W. CASTLEMAN Jr., University Park, PA
S.T. CEYER, Cambridge, MA
D. CHANDLER, Berkeley, CA
F.F. CRIM, Madison, WI
A. DALGARNO, Cambridge, MA
C.E. DYKSTRA, Indianapolis, IN
K.B. EISENTHAL, New York, NY
M.A. EL-SAYED, Atlanta, GA
M.D. FAYER, Stanford, CA
G.R. FLEMING, Chicago, IL
R.M. HOCHSTRASSER, Philadelphia, PA
J.L. KINSEY, Houston, TX
S.R. LEONE, Boulder, CO
M.I. LESTER, Philadephia, PA
W.C. LINEBERGER, Boulder, CO
B.V. McKOY, Pasadena, CA
W.H. MILLER, Berkeley, CA
K. MOROKUMA, Atlanta, GA
S. MUKAMEL, Rochester, NY
A. PINES, Berkeley, CA
A.R. RAVISHANKARA, Boulder, CO
S.A. RICE, Chicago, IL
P.J. ROSSKY, Austin, TX
R.J. SAYKALLY, Berkeley, CA
H.F. SCHAEFER III, Athens, GA
G.C. SCHATZ, Evanston, IL
R.E. SMALLEY, Houston, TX
W.C. STWALLEY, Storrs, CT
D.G. TRUHLAR, Minneapolis, MN
J.J. VALENTINI, New York, NY
G.M. WHITESIDES, Cambridge, MA
C. WITTIG, Los Angeles, CA
P.G. WOLYNES, Urbana, IL
J.T. YATES Jr., Pittsburgh, PA
R.N. ZARE, Stanford, CA

Contributions should, preferably, be sent to a member of the Advisory Editorial Board (addresses are given in the first issue of each volume) who is familiar with the research reported, or to one of the Editors:

A.D. BUCKINGHAM
D.A. KING
Editor of Chemical Physics Letters
University Chemical Laboratory
Lensfield Road
Cambridge CB2 1EW, UK
FAX 44-1223-336362

A.H. ZEWAIL
Editor of Chemical Physics Letters
A.A. Noyes Laboratory of Chemical Physics
California Institute of Technology
Mail Code 127-72
Pasadena, CA 91125, USA
FAX 1-818-4050454

After acceptance of the paper for publication, all further correspondence should be sent to the publishers (Ms. S.A. Hallink, Issue Management (Chemistry), Elsevier Science B.V., P.O. Box 2759, 1000 CT Amsterdam, The Netherlands; telephone 31-20-4852664, FAX 31-20-4852775, telex 10704 espom nl; electronic mail X400: C=NL; A=400NET; P=SURF; O=ELSEVIER; S=HALLINK, I=S or RFC822: S. HALLINK@ELSEVIER.NL).

Publication information: Chemical Physics Letters (ISSN 0009-2614). For 1997, volumes 264–280 are scheduled for publication. Subscription prices are available upon request from the publisher. Subscriptions are accepted on a prepaid basis only and are entered on a calendar year basis. Issues are sent by surface mail except to the following countries where Air delivery via SAL is ensured: Argentina, Australia, Brazil, Canada, Hong Kong, India, Israel, Japan, Malaysia, Mexico, New Zealand, Pakistan, PR China, Singapore, South Africa, South Korea, Taiwan, Thailand, USA. For all other countries airmail rates are available upon request. Claims for missing issues must be made within six months of our publication (mailing) date.

Copyright © 1997, Elsevier Science B.V. All rights reserved

0009-2614/1997/$17.00

US mailing notice – Chemical Physics Letters (ISSN 0009-2614) is published weekly by Elsevier Science B.V., Molenwerf 1, P.O. Box 211, 1000 AE Amsterdam. Annual subscription price in the USA US$ 7818.00, including air speed delivery, valid in North, Central and South America only. Periodicals postage paid at Jamaica, NY 11431. USA POSTMASTERS: Send address changes to Chemical Physics Letters, Publications Expediting, Inc., 200 Meacham Avenue, Elmont, NY 11003. Airfreight and mailing in the USA by Publication Expediting.

Printed in The Netherlands | Published weekly | Library of Congress Catalog Card Number 68–26532

CHEMICAL PHYSICS LETTERS

KEY GUIDELINES FOR AUTHORS

- All manuscripts require an abstract which should be informative and not exceed 100 words.
- The total number of references should not exceed 35; multiple references (containing more than one paper) should be avoided.
- The number of figures should not exceed 5 normal-sized figures.
- The manuscript should normally not exceed the equivalent of 2500 words including text, tables and figure captions (approximately 12 double-spaced pages).
- Authors are encouraged to submit a disk with an electronic file exactly matching the hard copy of their manuscript.
- Manuscripts should be sent to one of the editors or preferably to a member of the Advisory Editorial Board who is familiar with the research field. When submitting to an editor, authors are urged to suggest the names of three appropriate referees.

The complete Instructions to Authors are on the last pages of each volume.

EDITORS: A.D. BUCKINGHAM, D.A. KING, A.H, ZEWAIL
Assistant Editor: Dr. R. Kobayashi, Cambridge, UK

FOUNDING EDITORS: G.J. HOYTINK, L. JANSEN
FORMER EDITORS: R.B. BERNSTEIN, D.A. SHIRLEY, R.N. ZARE

ADVISORY EDITORIAL BOARD

Australia
B.J. ORR, Sydney

Canada
P.A. HACKETT, Ottawa
J.W. HEPBURN, Waterloo
C.A. McDOWELL, Vancouver

Czech Republic
Z. HERMAN, Prague

Denmark
F. BESENBACHER, Aarhus
G.D. BILLING, Copenhagen

France
E. CLEMENTI, Strasbourg
J. DURUP, Toulouse
J.-M. LEHN, Strasbourg
J.-L. MARTIN, Palaiseau
B. SOEP, Orsay

Germany
R. AHLRICHS, Karlsruhe
V.E. BONDYBEY, Garching
W. DOMCKE, Dusseldorf
G. ERTL, Berlin
G. GERBER, Würzburg
G.L. HOFACKER, Garching
D.M. KOLB, Ulm
J. MANZ, Berlin
M. PARRINELLO, Stuttgart
S.D. PEYERIMHOFF, Bonn
R. SCHINKE, Göttingen
E.W. SCHLAG, Garching
J. TROE, Göttingen
H.C. WOLF, Stuttgart
W. ZINTH, Munich

India
C.N.R. RAO, Bangalore

Israel
J. JORTNER, Tel Aviv
R.D. LEVINE, Jerusalem

Italy
V. AQUILANTI, Perugia

Japan
H. HAMAGUCHI, Tokyo
M. ITO, Okazaki
T. KOBAYASHI, Tokyo
K. KUCHITSU, Sakado
H. NAKATSUJI, Kyoto
K. TANAKA, Tokyo
K. YOSHIHARA, Ishikawa

People's Republic of China
C.-H. ZHANG, Beijing

Poland
Z.R. GRABOWSKI, Warsaw

Russian Federation
A.L. BUCHACHENKO, Moscow
V.S. LETOKHOV, Troitzk
Yu.N. MOLIN, Novosibirsk

Spain
A. GONZÁLEZ UREÑA, Madrid

Sweden
P.E.M. SIEGBAHN, Stockholm
V. SUNDSTRÖM, Lund

Switzerland
M. CHERGUI, Lausanne-Dorigny
R.R. ERNST, Zurich
M. QUACK, Zurich

Taiwan, ROC
Y.T. LEE, Taipei

The Netherlands
A.J. HOFF, Leiden
A.W. KLEYN, Amsterdam
D.A. WIERSMA, Groningen

United Kingdom
M.N.R. ASHFOLD, Bristol
G.S. BEDDARD, Leeds
M.S. CHILD, Oxford
D.C. CLARY, London
R. FREEMAN, Cambridge
R.H. FRIEND, Cambridge
N.C. HANDY, Cambridge
A.C. LEGON, Exeter
R.M. LYNDEN-BELL, Belfast
J.P. SIMONS, Oxford
I.W.M. SMITH, Birmingham

USA
P. AVOURIS, Yorktown Heights, NY
A.J. BARD, Austin, TX
A.W. CASTLEMAN Jr., University Park, PA
S.T. CEYER, Cambridge, MA
D. CHANDLER, Berkeley, CA
F.F. CRIM, Madison, WI
A. DALGARNO, Cambridge, MA
C.E. DYKSTRA, Indianapolis, IN
K.B. EISENTHAL, New York, NY
M.A. EL-SAYED, Atlanta, GA
M.D. FAYER, Stanford, CA
G.R. FLEMING, Chicago, IL
R.M. HOCHSTRASSER, Philadelphia, PA
J.L. KINSEY, Houston, TX
S.R. LEONE, Boulder, CO
M.I. LESTER, Philadelphia, PA
W.C. LINEBERGER, Boulder, CO
B.V. McKOY, Pasadena, CA
W.H. MILLER, Berkeley, CA
K. MOROKUMA, Atlanta, GA
S. MUKAMEL, Rochester, NY
A. PINES, Berkeley, CA
A.R. RAVISHANKARA, Boulder, CO
S.A. RICE, Chicago, IL
P.J. ROSSKY, Austin, TX
R.J. SAYKALLY, Berkeley, CA
H.F. SCHAEFER III, Athens, GA
G.C. SCHATZ, Evanston, IL
R.E. SMALLEY, Houston, TX
W.C. STWALLEY, Storrs, CT
D.G. TRUHLAR, Minneapolis, MN
J.J. VALENTINI, New York, NY
G.M. WHITESIDES, Cambridge, MA
C. WITTIG, Los Angeles, CA
P.G. WOLYNES, Urbana, IL
J.T. YATES Jr., Pittsburgh, PA
R.N. ZARE, Stanford, CA

CHEMICAL PHYSICS LETTERS

Editors

DAVID BUCKINGHAM, Cambridge

DAVID KING, Cambridge

AHMED ZEWAIL, Pasadena

MASTER INDEX VOLUMES 261–270
OCTOBER 1996 – MAY 1997

ELSEVIER
Amsterdam – Lausanne – New York – Oxford – Shannon – Tokyo

Copyright © 1997, Elsevier Science B.V. All rights reserved 0009-2614/1997/$17.00

This journal and the individual contributions contained in it are protected by the copyright of Elsevier Science B.V., and the following terms and conditions apply to their use:

Photocopying
Single photocopies of single articles may be made for personal use as allowed by national copyright laws. Permission of the Publisher and payment of a fee is required for all other photocopying, including multiple or systematic copying, copying for advertising or promotional purposes, resale, and all forms of document delivery. Special rates are available for educational institutions that wish to make photocopies for non-profit educational classroom use.
In the USA, users may clear permissions and make payment through the Copyright Clearance Center Inc., 222 Rosewood Drive, Danvers, MA 01923, USA; Tel. (508)7508400; Fax (508)7504744. In the UK, users may clear permissions and make payment through the Copyright Licensing Agency Rapid Clearance Service (CLARCS), 90 Tottenham Court Road, London W1P 0LP, UK. In other countries where a local copyright clearance centre exists, please contact it for information on required permissions and payments.

Derivative Works
Subscribers may reproduce tables of contents or prepare lists of articles including abstracts for internal circulation within their institutions. Permission of the Publisher is required for resale or distribution outside the institution.
Permission of the Publisher is required for all other derivative works, including compilations and translations.

Electronic Storage
Permission of the Publisher is required to store electronically any material contained in this journal, including any article or part of an article. Contact the Publisher at the address indicated.

Except as outlined above, no part of this publication may be reproduced, stored in a retrieval system or transmitted in any form or by any means, electronic, mechanical, photocopying, recording or otherwise, without prior written permission of the Publisher.

Disclaimer
No responsibility is assumed by the Publisher for any injury and/or damage to persons or property as a matter of products liability, negligence or otherwise, or from any use or operation of any methods, products, instructions or ideas contained in the material herein.

Although all advertising material is expected to conform to ethical (medical) standards, inclusion in this publication does not constitute a guarantee or endorsement of the quality or value of such product or of the claims made of it by its manufacturer.

Elsevier Science B.V.
Tel: (+31-20)4852-664 Fax: (+31-20)4852-775 E-mail: s.hallink@elsevier.nl

Postal Address

Elsevier Science B.V.
P.O. Box 2759
1000 CT Amsterdam
The Netherlands

Courier Service Address

Elsevier Science B.V.
Sara Burgerhartstraat 25
1055 KV Amsterdam
The Netherlands

Printed in The Netherlands

∞ The paper used in this publication meets the requirements of ANSI/NISO Z39.48-1992 (Permanence of Paper).

ELSEVIER

June 1997

Chemical Physics Letters 261–270 (1997) v–x

CHEMICAL PHYSICS LETTERS

List of advisory editors

Professor Dr. R. Ahlrichs, Lehrstuhl für Theoretische Chemie, Universität Karlsruhe, D-76128 Karlsruhe, Germany. FAX 49-721-6084856

Professor V. Aquilanti, Dipartimento di Chimica dell'Università, via Elce di Sotto 8, 06100 Perugia, Italy. FAX 39-75-5855606

Professor M.N.R. Ashfold, School of Chemistry, University of Bristol, Cantock's Close, Bristol BS8 1TS, UK. FAX 44-117-9250612

Dr. P. Avouris, IBM Research Division, T.J. Watson Research Center, P.O. Box 218, Route 134, Yorktown Heights, NY 10598, USA. FAX 1-914-9452141

Professor A.J. Bard, Hackerman/Welch Regents Chair in Chemistry, Department of Chemistry, The University of Texas at Austin, Austin, TX 78712-1167, USA. FAX 1-512-4710088

Dr. G.S. Beddard, School of Chemistry, University of Leeds, Leeds LS2 9JT, UK. godfrey.beddard@chem.leeds.ac.uk

Professor F. Besenbacher, Institute of Physics and Astronomy, University of Aarhus, DK-8000 Aarhus, Denmark. FAX 45-86-120740

Professor Dr. V.E. Bondybey, Institut für Physikalische und Theoretische Chemie der Technischen Universität München, Lichtenbergstrasse 4, D-85748 Garching near Munich, Germany. FAX 49-89-32092727

Professor A.L. Buchachenko, N.N. Semenov Institute of Chemical Physics, Russian Academy of Sciences, Ulitsa Kosygina 4, 117334 Moscow, Russian Federation. FAX 7-095-9382156

Professor A.W. Castleman Jr., Department of Chemistry, Pennsylvania State University, 152 Davey Laboratory, University Park, PA 16802, USA. FAX 1-814-8655235

Professor L.S. Cederbaum, Theoretische Chemie, Institut für Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, D-69120 Heidelberg, Germany. FAX 49-6221-565221

Dr. Y. Chabal, AT&T Bell Laboratories, Room 1C-462, Murray Hill, NJ 07974-2070, USA. FAX 1-908-5823901

Professor D. Chandler, Department of Chemistry, University of California, Berkeley, CA 94720, USA. FAX 1-510-6428369

Professor M. Chergui, Institut de Physique Experimentale, Université de Lausanne, BSP, CH-1015 Lausanne-Dorigny, Switzerland. FAX 41-21-6923635

Professor M.S. Child, Physical and Theoretical Chemistry Laboratory, University of Oxford, 5 South Parks Road, Oxford OX1 3UB, UK. FAX 44-1865-275410

Professor D.C. Clary, Department of Chemistry, University College London, London WC1H OAJ, UK. FAX 44-171-380-7463

Professor E. Clementi, Laboratoire M.E.T.E.C.C., Institut de Physique, Université Louis Pasteur, 3 rue de l'Université, 67084 Strasbourg Cedex, France, FAX 33-88-358191

Professor F.F. Crim, Department of Chemistry, University of Wisconsin at Madison, 1101 University Avenue, Madison, WI 53706, USA. FAX 1-608-2629918

Professor A. Dalgarno, F.R.S., Harvard College Observatory and Smithsonian Astrophysical Observatory, 60 Garden Street, Cambridge, MA 02138, USA. FAX 1-617-4955970

Dr. P.M. Dehmer, Argonne National Laboratory, Building 203-B161, Argonne, IL 60439, USA. FAX 1-708-2527415

Professor J. Durup, IRSAMC, 118, route de Narbonne, 31062 Toulouse, France. FAX 33-61-556065

Professor C.E. Dykstra, Department of Chemistry, School of Science, IUPUI, 402 N. Blackford Street, Indianapolis, IN 46205, USA. FAX 1-317-2744701

Professor K.B. Eisenthal, Department of Chemistry, Columbia University, Havemeyer Hall, 116th Street and Broadway, New York, NY 10027, USA. FAX 1-212-9321289

Professor M.A. El-Sayed, School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA 30332-0400, USA. FAX 1-404-8940294

Professor Dr. R.R. Ernst, Laboratorium für Physikalische Chemie, ETH Zentrum, CH-8092 Zurich, Switzerland. FAX 41-1-2523402

Professor Dr. G. Ertl, Department of Physical Chemistry, Fritz-Haber Institut der Max-Planck Gesellschaft, Faradayweg 4-6, D-14195 Berlin (Dahlem), Germany. FAX 49-308-305520

Professor M.D. Fayer, Department of Chemistry, Stanford University, Stanford, CA 94305, USA. FAX 1-415-7250259

Professor G.R. Fleming, Department of Chemistry, University of Chicago, 5735 South Ellis Avenue, Chicago, IL 60637, USA. FAX 1-312-7020805

Professor R. Freeman, Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, UK. FAX 44-1223-336362

Dr. R.H. Friend, F.R.S., Cavendish Laboratory, University of Cambridge, Madingley Road, Cambridge CB3 0HE, UK. FAX 44-1223-63263

Professor G. Gerber, Physikalisch Institut der Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany. FAX 49-931-8884906

Professor A. González Ureña, Instituto Pluridisciplinar, Juan XXIII-1, Universidad Complutense, 28040 Madrid, Spain. FAX 34-1-3943265

Professor D.W. Goodman, Department of Chemistry, Texas A&M University, College Station, TX 77843-3255, USA. FAX 1-409-8456822

Professor Dr. Z.R. Grabowski, Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44, 01-224 Warsaw, Poland. FAX 48-39-120238

Professor P.A. Hackett, Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa, Canada K1A 0R6. FAX 1-613-9545242

Professor H. Hamaguchi, Department of Chemistry, School of Science, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113, Japan. FAX 81-3-38184621

Professor N.C. Handy, F.R.S., University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, UK. FAX 44-1223-336362

Professor J.W. Hepburn, Department of Chemistry, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1. FAX 1-519-7460435

Dr. Z. Herman, J. Heyrovsky Institute of Physical Chemistry and Electrochemistry, Academy of Sciences of the Czech Republic, Dolcjškova 3, 182 23 Prague 8, Czech Republic. FAX 42-2-8582307

Professor R.M. Hochstrasser, Department of Chemistry/D5, University of Pennsylvania, Philadelphia, PA 19104, USA. FAX 1-215-8980590

Professor Dr. G.L. Hofacker, Lehrstuhl für Theoretische Chemie, Technische Universität München, Lichtenbergstrasse 4, D-85747 Garching near Munich, Germany. FAX 49-89-32093622

Professor Dr. A.J. Hoff, Department of Biophysics, Huygens Laboratorium, Rijksuniversiteit te Leiden, Postbus 9504, 2300 RA Leiden, The Netherlands. FAX 31-71-275819

Professor M. Ito, Institute for Molecular Science, Myodaiji, Okazaki 444, Japan. FAX 81-564-542254

Professor J. Jortner, Institute of Chemistry, Tel-Aviv University, 61390 Ramat Aviv, Tel Aviv, Israel. FAX 972-3-6415054

Professor J.L. Kinsey, Dean and D.R. Bullard-Welch Foundation Professor of Science, Wiess School of Natural Sciences, Rice University, P.O. Box 1892, Houston, TX 77251, USA. FAX 1-713-2855401

Professor A.W. Kleyn, FOM-Instituut voor Atoom- en Molekuulfysica, Kruislaan 407, 1098 SJ Amsterdam, The Netherlands. FAX 31-20-6684106

Professor T. Kobayashi, Department of Physics, Faculty of Science, University of Tokyo, 7-3-1 Hongo, Bunkyo ku, Tokyo 113, Japan. FAX 81-3-38187812

Professor Dr. D.M. Kolb, Abt. Elektrochemie, Universität Ulm, D-89069 Ulm, Germany. FAX 49-731-5025409

Professor K. Kuchitsu, Department of Chemistry, Josai University, Keyakidai, Sakado 350-02, Japan. FAX 81-492-717985

Professor Y.T. Lee, Academia Sinica, Taipei 11529, Taiwan, ROC. FAX 886-2-7853852

Professor A.C. Legon, Department of Chemistry, University of Exeter, Stocker Road, Exeter EX4 4QD, UK. FAX 44-1392-263434

Professor J.-M. Lehn, Laboratoire de Chimie Supramoleculaire, Université Louis Pasteur, 4, rue Blaise Pascal, 67000 Strasbourg, France. FAX 33-88-411020

Professor S.R. Leone, Division of Chemistry, Join Institute for Laboratory Astrophysics, Campus Box 440, University of Colorado, Boulder, CO 80309, USA. FAX 1-303-4925235

Professor V.S. Letokhov, Institute of Spectroscopy, Russian Academy of Sciences, 142092 Troitzk, Moscow Region, Russian Federation

Professor R.D. Levine, Department of Physical Chemistry, The Hebrew University of Jerusalem, Jerusalem 91904, Israel. FAX 972-2-513742

Professor C.M. Lieber, Department of Chemistry, Harvard University, 12 Oxford Street, Cambridge, MA 02138, USA. FAX 1-617-4965442

Professor W.C. Lineberger, Department of Chemistry and JILA, Box 440, University of Colorado, Boulder, CO 80309, USA. FAX 1-303-4928994

Dr. R.M. Lynden-Bell, School of Mathematics and Physics, The Queen's University, Belfast BT7 1NN, Northern Ireland, UK. Fax 44-1232-239182

Professor Dr. J. Manz, Fachbereich Chemie, Institut für Physikalische und Theoretische Chemie, Freie Universität Berlin, Takustrasse 3, D-14195 Berlin, Germany. FAX 49-30-8384792

Professor J.-L. Martin, Laboratoire d'Optique Appliquée, INSERM U 275, Ecole Polytechnique, CNRS URA 1406, ENSTA – Centre de l'Yvette, 91128 Palaiseau, France. FAX 33-1-60106085

Professor C.A. McDowell, Department of Chemistry, University of British Columbia, 2036 Main Mall, Vancouver 8, British Columbia, Canada V6T 1Y6. FAX 1-604-8222847

Professor B.V. McKoy, Division of Chemistry and Chemical Engineering, The Chemical Laboratories, California Institute of Technology, Pasadena, CA 91125, USA. FAX 1-818-5777715

Professor W.H. Miller, Department of Chemistry, University of California, Berkeley, CA 94720, USA. FAX 1-510-6428369

Professor Yu.N. Molin, Institute of Chemical Kinetics and Combustion, Academy of Science, 630090 Novosibirsk, Russian Federation. FAX 7-3832-352350

Professor K. Morokuma, Department of Chemistry, Emory University, Atlanta, GA 30322, USA. FAX 1-404-7276586

Professor S. Mukamel, Department of Chemistry, University of Rochester, Rochester, NY 14627, USA. FAX 1-716-4736889

Professor H. Nakatsuji, Department of Synthetic Chemistry, Faculty of Engineering, Sakyo-Ku, Kyoto 606-01, Japan. FAX 81-75-7535910

Professor J.K. Nørskov, Physics Department, Building 307, Technical University of Denmark, DK-2800 Lyngby, Denmark. FAX 45-45-932399

Professor B.J. Orr, School of Chemistry, Macquarie University, Sydney, NSW 2109, Australia. FAX 61-2-8508313

Professor M. Parrinello, Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70506 Stuttgart, Germany. FAX 49-711-6891702.

Professor Dr. S.D. Peyerimhoff, Lehrstuhl für Theoretische Chemie der Universität Bonn, Wegelerstrasse 12, D-53115 Bonn 1, Germany. FAX 49-228-732557

Professor A. Pines, Department of Chemistry, University of California, Berkeley, CA 94720, USA. FAX 1-510-6428369

Professor Dr. M. Quack, Laboratorium für Physikalische Chemie, ETH-Zentrum, CH-8092 Zurich, Switzerland. FAX 41-1-6321021

Professor C.N.R. Rao, F.R.S., Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore 560012, India. FAX 91-80-341683

Dr. A.R. Ravishankara, NOAA, Environmental Laboratories, Mail stop R/E/AL2, 325 Broadway, Boulder, CO 80303-3328, USA. FAX 1-303-4975822

Professor S.A. Rice, Department of Chemistry, The James Franck Institute, The University of Chicago, 5640 Ellis Avenue, Chicago, IL 60637, USA. FAX 1-312-7025863

Professor P.J. Rossky, Department of Chemistry & Biochemistry, University of Texas at Austin, Austin, TX 78712-1167, USA. FAX 1-512-4711624

Professor R.J. Saykally, Department of Chemistry, University of California, Berkeley, CA 94720, USA. FAX 1-510-6428369

Professor H.F. Schaefer III, Center for Computational Quantum Chemistry, University of Georgia, Athens, GA 30602, USA. FAX 1-404-5420406

Professor G.C. Schatz, Department of Chemistry, Northwestern University, 2145 Sheridan Road, Evanston, IL 60208, USA. FAX 1-708-4672447

Dr. R. Schinke, Max-Planck Institut für Strömungsforschung, Postfach 2853, D-37073 Göttingen, Germany. FAX 49-551-7092607

Professor E.W. Schlag, Lehrstuhl für Physikalische Chemie I, Technische Universität München, Lichtenbergstrasse 4, D-85747 Garching near Munich, Germany. FAX 49-89-32093389

Professor P.E.M. Siegbahn, Stockholms Universitet, Fysikum, Vanadisvägen 9, S-113 46 Stockholm, Sweden. FAX 46-8-347817

Professor J.P. Simons, F.R.S., Physical Chemistry Laboratory, University of Oxford, South Parks Road, Oxford OX1 3QZ, UK. FAX 44-1865-275410

Professor R.E. Smalley, Department of Chemistry, Rice University, Houston, TX 77001, USA. FAX 1-713-2855155

Professor I.W.M. Smith, Department of Chemistry, University of Birmingham, Edgbaston, Birmingham B15 2TT, UK. FAX 44-121-4144403

Dr. B. Soep, Laboratoire de Photophysique Moléculaire, Bâtiment 213, Université de Paris Sud, 91405 Orsay, France. FAX 33-1-69416777

Professor W.C. Stwalley, Department of Physics, University of Connecticut, 2152 Hillside Road, U-46, Storrs, CT 06269-3046, USA. FAX 1-203-4863346

Professor V. Sundström, Chemical Dynamics and Spectroscopy, Lund University, P.O. Box 124, S-221 00 Lund, Sweden. FAX 46-46-104119

Professor K. Tanaka, The Institute for Solid State Physics, The University of Tokyo, 7-22-1 Roppongi, Minatoku, Tokyo 106, Japan. FAX 81-3-34015169

Professor J. Troe, Institut für Physikalische Chemie der Universität, Tammannstrasse 6, D-37077 Göttingen, Germany. FAX 49-551-393144

Professor D.G. Truhlar, Department of Chemistry, University of Minnesota, Minneapolis, MN 55455, USA. FAX 1-612-6269390

Professor J.J. Valentini, Department of Chemistry, Columbia University, New York, NY 10027, USA. FAX 1-212-9321289

Professor H. Walther, Max-Planck-Institut für Quantenoptik, Ludwig-Prandtl-Strasse 10, D-85748 Garching, Germany. FAX 49-89-32905710

Professor D.A. Wiersma, Department of Chemistry, Ultrafast Laser and Spectroscopy Laboratory, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands. FAX 31-50-634441

Professor C. Wittig, Department of Chemistry, University of Southern California, Los Angeles, CA 90089, USA. FAX 1-213-7402701

Professor Dr. H.C. Wolf, Physikalisches Institut der Universität, Pfaffenwaldring 57, D-70550 Stuttgart 80, Germany. FAX 49-711-6855281

Dr. P.G. Wolynes, University of Illinois, School of Chemical Sciences, 505 South Mathews Avenue, Urbana, IL 61801, USA. FAX 1-217-2448068

Professor K. Yoshihara, Department of Materials Science, Japan Advanced Institute of Science and Technology, Tatsonokuchi, Ishikawa 923-12, Japan. FAX 81-761511149

Professor R.N. Zare, Department of Chemistry, Stanford University, Stanford, CA 94305, USA. FAX 1-415-7250259

Professor C.-H. Zhang, National Natural Science Foundation of China, 35 Huayuan Beilu, East Gate, Haidian District, Beijing 100083, People's Republic of China. FAX 86-1-2010306

June 1997

ELSEVIER

Chemical Physics Letters 261–270 (1997) 1–96

CHEMICAL PHYSICS LETTERS

Author index to volumes 261–270

Aartsma, T.J., see Streltsov, A.M. 266 (1997) 347
Abbate, F., see Lanzani, G. 264 (1997) 667
Abbate, M., see Soriano, L. 266 (1997) 184
Abboud, J.L.M., see Notario, R. 263 (1996) 367
Abe, H., see Nishizawa, K. 267 (1997) 501
Abe, J., N. Nemoto, Y. Nagase and Y. Shirai, Ab initio MO investigations of molecular structures in the ground and first excited states of heterocyclic pyridinium betaine 261 (1996) 18
Abergel, D., A. Louis-Joseph and J.-Y. Lallemand, A new concept for selective excitation in NMR 262 (1996) 465
Abou-Zied, O.K., D.R.M. Demmer, S.C. Wallace and R.P. Steer, Picosecond dynamics of the S_2 excited state of azulene and its van der Waals complexes with Ar and Xe 266 (1997) 75
Achatz, U., see Albert, G. 268 (1997) 235
Achiba, Y., see Qin, L.-C. 268 (1997) 101
Adamčíková, L., see Ševčík, P. 267 (1997) 307
Adamo, C., V. Dillet and V. Barone, Solvent effects on the conformational behavior of model peptides. A comparison between different continuum models 263 (1996) 113
Adamo, C. and P. Maldivi, Ionic versus covalent character in lanthanide complexes. A hybrid density functional study 268 (1997) 61
Adamowicz, L., see Elkadi, Y. 261 (1996) 507
Adamowicz, L., see Smets, J. 262 (1996) 789
Adamson, R.D., see Gill, P.M.W. 261 (1996) 105
Adelmann, P., see Cummins, T.R. 261 (1996) 228
Adhikari, S. and S.P. Bhattacharyya, A fast iterative route to the optimal angle of rotation in the complex coordinate rotation method: some model applications 265 (1997) 99
Adhikari, S., New propagator schemes for explicitly time-dependent Hamiltonians: applications to the multiphoton dissociation dynamics of diatoms 262 (1996) 526
Adhikari, S.K. and A.S. Ghosh, Positron–helium scattering at medium energies 262 (1996) 460
Agafonov, V., V.A. Davydov, L.S. Kashevarova, A.V. Rakhmanina, A. Kahn-Harari, P. Dubois, R. Céolin and H. Szwarc, 'Low-pressure' orthorhombic phase formed from pressure-treated C_{60} 267 (1997) 193
Agmon, N., see Zaloj, V. 270 (1997) 476
Agrawal, P.M., N.K. Dabkara and S. Tilwankar, Rotational energy transfer in the NO–Ar system and the validity of the different forms of the potential 266 (1997) 481
Ågren, H., see Norman, P. 268 (1997) 337
Aguilar, A., see Romero, T. 261 (1996) 583
Ahlrichs, R., see Bauernschmitt, R. 264 (1996) 573
Ajayan, P.M., see Banhart, F. 269 (1997) 349

Akasaka, T., see Kobayashi, K. 261 (1996) 502
Åkerlund, C., I. Zorić, B. Kasemo, A. Cupolillo, F. Buatier de Mongeot and M. Rocca, Dissociation of O_2 chemisorbed on Ag (110) and Pt(111) induced by energetic Xe atoms 270 (1997) 157
Akhmatskaya, E.V., M.D. Cooper, N.A. Burton, A.J. Masters and I.H. Hillier, Monte Carlo simulations of water clusters on a parallel computer using an ab initio potential 267 (1997) 105
Akimoto, Y., see Harima, Y. 267 (1997) 481
Akimov, A.V., see Goldschleger, A.U. 267 (1997) 288
Akiyama, K., see Sekiguchi, S. 263 (1996) 161
Akiyama, T., see Imahori, H. 263 (1996) 545
Al-Omari, A.K., see Altmann, K.N. 261 (1996) 597
Ala-Korpela, M., see Hyvönen, M. 268 (1997) 55
Alanko, S., see Ulenikov, O.N. 268 (1997) 242
Albert, G., C. Berg, M. Beyer, U. Achatz, S. Joos, G. Niedner-Schatteburg and V.E. Bondybey, Methane activation by rhodium cluster argon complexes 268 (1997) 235
Albertí, M., see Romero, T. 261 (1996) 583
Albrecht, A.C., see Stimson, M.J. 263 (1996) 185
Aleinikov, N.N., G.K. Vasiliev, S.A. Kashtanov, E.F. Makarov and Yu.A. Chernishev, Absorption cross sections and products of photodissociation of xenon tetroxide 267 (1997) 155
Alekseyev, A.B., see Wright, J.S. 266 (1997) 391
Alexander, A.J., F.J. Aoiz, M. Brouard, I. Burak, Y. Fujimura, J. Short and J.P. Simons, An experimental and quasiclassical study of the product state resolved stereodynamics of the reaction $O(^1D_2) + H_2(v = 0) \rightarrow OH(X^2\Pi_{3/2};\ v = 0,\ N,\ f) + H$ 262 (1996) 589
Alexandrov, A.L. and V.A. Schweigert, A kinetic model of carbon cluster growth including polycyclic rings and fullerene formation 263 (1996) 551
Alford, J.M., see Ding, X. 269 (1997) 72
Ali, S.S., K. Maeda, H. Murai and T. Azumi, Surprisingly large magnetic field effect in the electron-transfer reaction of 4,4′-bipyridine with triethylamine in acetonitrile 267 (1997) 520
Allan, M. and D.B. Popović, Vibronic coupling and selectivity of vibrational excitation in the negative ion resonances of ozone 268 (1997) 50
Allavena, M., see Šepa, J. 262 (1996) 321
Allen, M.D., B.Z. Li and L.M. Ziurys, A millimeter/sub-millimeter-wave spectroscopic study of the FeCl radical ($X\ ^6\Delta_i$) 270 (1997) 517
Allen, T.M., see Russell, T.P. 267 (1997) 351
Allouche, A.-R., see Antoine, R. 261 (1996) 670
Aloisi, G.G., see Holmes, A.S. 266 (1997) 309
Altmann, K.N., A.K. Al-Omari and R. Reininger, Field ionization of Wannier excitons in liquid xenon 261 (1996) 597
Alvarez, M.M., J.T. Khoury, T.G. Schaaff, M. Shafigullin, I. Vezmar and R.L. Whetten, Critical sizes in the growth of Au clusters 266 (1997) 91
Alvarez-Ramirez, J., R. Martinez and E. Díaz-Herrera, Solution of the Poisson–Boltzmann equation through the use of pseudo-dynamic simulation method 266 (1997) 375
Alvira, E., Physisorption in cyclodextrin cavities: an analytical model 267 (1997) 221
Amatatsu, Y., see Dzegilenko, F.N. 264 (1997) 24
Amaya, K., see Teki, Y. 270 (1997) 573
Ambrose, W.P., P.M. Goodwin, J. Enderlein, D.J. Semin, J.C. Martin and R.A. Keller, Fluorescence photon antibunching from single molecules on a surface 269 (1997) 365
Ambrose, W.P., see Enderlein, J. 270 (1997) 464
Amekraz, B., see Luna, A. 266 (1997) 31

Ameloot, M., see Molski, A. 266 (1997) 139
Amijima, Y., see Hamanoue, K. 267 (1997) 165
Andersen, J.N., A. Beutler, S.L. Sorensen, R. Nyholm, B. Setlik and D. Heskett, Vibrational fine structure in the C 1s core level photoemission of chemisorbed molecules: ethylene and ethylidyne on Rh(111) 269 (1997) 371
Anderson, A., W. Smith and J.F. Wheeldon, Infrared study of sulphur at high pressures 263 (1996) 133
Anderson, A., see Lee, S.A. 262 (1996) 337
Anderson, A., see Eaton, R.A. 269 (1997) 309
Anderson, A., see Yuan, Y.N.F. 269 (1997) 305
Anderson, H.L., see Piet, J.J. 266 (1997) 70
Anderson, J.B., see Mella, M. 265 (1997) 467
Andersson, M.R., see Schwartz, B.J. 265 (1997) 327
Andreasson, B., see van Dam, L. 262 (1996) 737
Andreev, D.V., see Makarshin, L.L. 266 (1997) 173
Andreoni, W., see Boero, M. 265 (1997) 24
Andreoni, W., see Grönbeck, H. 269 (1997) 385
Andrews, P.M., B.A. Pryor, P.M. Palmer and M.R. Topp, Structural measurements of hydrogen-bonded complexes of perylene with water and methanol 265 (1997) 224
Andrews, P.M., see Pryor, B.A. 267 (1997) 531
Andrews, S.B., N.A. Burton, I.H. Hillier, J.M. Holender and M.J. Gillan, Molecular electronic structure calculations employing a plane wave basis: a comparison with Gaussian basis calculations 261 (1996) 521
Andrews, S.B., N.A. Burton and I.H. Hillier, A stepwise reaction path for the homolytic chemisorption of H_2 onto the MgO (100) surface 269 (1997) 475
Andrews, S.R., see Silcocks, S.E. 262 (1996) 355
Anglada, J.M. and J.M. Bofill, A symmetric orthogonal transformation applied to molecular geometry optimizations constrained on a hypersphere 269 (1997) 469
Anishchik, S.V., see Borovkov, V.I. 270 (1997) 327
Anisimov, O.A., see Borovkov, V.I. 270 (1997) 327
Antoine, R., Ph. Dugourd, D. Rayane, A.-R. Allouche, M. Aubert-Frécon and M. Broyer, On the optical absorption spectrum of Li_2H 261 (1996) 670
Antonova, S., K. Urbanski, A.M. Lyyra, F.C. Spano and L. Li, State to state collision energy transfer in singlet states of Li_2 267 (1997) 158
Anttila, R., see Ulenikov, O.N. 268 (1997) 242
Aoiz, F.J., L. Bañares, V.J. Herrero, V. Sáez Rábanos, K. Stark, I. Tanarro and H.-J. Werner, The F + HD reaction: cross sections and rate constants on an ab initio potential energy surface 262 (1996) 175
Aoiz, F.J., M. Brouard, V.J. Herrero, V. Sáez Rábanos and K. Stark, Product rotational polarization. The stereodynamics of the $F + H_2$ reaction 264 (1997) 487
Aoiz, F.J., see Alexander, A.J. 262 (1996) 589
Aoiz, F.J., see Wrede, E. 265 (1997) 129
Aoki, M., see Imahori, H. 263 (1996) 545
Aquilanti, V. and J. Avery, Generalized potential harmonics and contracted Sturmians 267 (1997) 1
Aquilanti, V., see de Castro Vítores, M. 263 (1996) 456
Arabei, S.M., J.P. Galaup and P. Jardon, Analysis of the site selected fluorescence and the phosphorescence spectrum of hypericin in ethanol 270 (1997) 31
Araki, Y., see Maeda, K. 262 (1996) 110
Aratono, Y., see Kumada, T. 261 (1996) 463

Aratono, Y., see Komaguchi, K. 268 (1997) 493
Arden-Jacob, J., see Müller, R. 262 (1996) 716
Aree, T. and S. Hannongbua, Ab initio study of collisions between Li and C_{60} 266 (1997) 427
Argyrakis, P., D.M. Basko, M.A. Drobizhev, A.N. Lobanov, A.V. Pimenov, O.P. Varnavsky, M. Van der Auweraer and A.G. Vitukhnovsky, Absorption lineshape of J-aggregates of thiacarbocyanine dyes: experiment and numerical study 268 (1997) 372
Arias, A.A., see Wasserman, T.A.W. 262 (1996) 329
Arita, K., see Lee, S. 265 (1997) 579
Armbruster, J.F., see Cummins, T.R. 261 (1996) 228
Arusi-Parpar, T., R.P. Schmid, R.-J. Li, I. Bar and S. Rosenwaks, Rotational-state dependent selectivity in the bond fission of $C_2^-HD\,(5\nu_1)$ 268 (1997) 163
Asai, S., see Suzuki, Y. 268 (1997) 213
Asai, T., see Umemoto, H. 264 (1997) 215
Aschi, M. and F. Grandinetti, Gaseous protonated nitrosamide. A G2 theoretical study on the structure, stability, and interconversion of $(H_2N\text{-}NO)H^+$ isomers 267 (1997) 98
Ashfold, M.N.R., J. Pearson, J.W. Hudgens and R.D. Johnson III, Resonance enhanced multiphoton ionisation of the SiF radical: a reinvestigation 263 (1996) 138
Ashfold, M.N.R., see Johnson III, R.D. 261 (1996) 474
Ashfold, M.N.R., see Wheeler, M.D. 268 (1997) 421
Asmus, K.-D., see Staško, A. 262 (1996) 233
Asselin, P., B. Dupuis, J.P. Perchard and P. Soulard, The gas phase infrared spectrum of HCl complexed with dimethyl ether revisited: assignment of the fundamental transition from a jet-cooled experiment 268 (1997) 265
Assfeld, X. and J.-L. Rivail, Quantum chemical computations on parts of large molecules: the ab initio local self consistent field method 263 (1996) 100
Au, C.T., M.-S. Liao and C.F. Ng, A theoretical investigation of methane dissociation of Rh(111) 267 (1997) 44
Aubert-Frécon, M., see Antoine, R. 261 (1996) 670
Avery, J., see Aquilanti, V. 267 (1997) 1
Aycard, J.P., see Bahou, M. 265 (1997) 145
Azria, R., see Hedhili, M.N. 268 (1997) 21
Azumi, T., see Ali, S.S. 267 (1997) 520
Azumi, T., see Maeda, K. 262 (1996) 110
Azumi, T., see Murai, H. 264 (1997) 619

Bacchiocchi, C. and C. Zannoni, Energy transfer in condensed systems. The effect of phase organization 268 (1997) 541
Bach, H., A. Renn and U.P. Wild, Excitation induced frequency shifts of single molecules 266 (1997) 317
Bach, R.D., see Glukhovtsev, M.N. 265 (1997) 514
Bach, R.D., see Hass, K.C. 263 (1996) 414
Bach, R.D., see Glukhovtsev, M.N. 269 (1997) 145
Bačić, Z., see Sabo, D. 261 (1996) 318
Backstrand, K.M., see Hain, T.D. 262 (1996) 723
Baddeley, C.J., see Lomas, J.R. 263 (1996) 591
Bae, S.C., G.H. Kim and J.K. Ku, Relaxation kinetics on the first excited singlet state of SO_2 from time resolved emission spectra 265 (1997) 385
Baer, M. and R. Englman, A modified Born–Oppenheimer equation: application to conical intersections and other types of singularities 265 (1997) 105

Baer, M., see Charutz, D.M. 265 (1997) 629
Baer, R., see Charutz, D.M. 265 (1997) 629
Baer, T., see Mayer, P.M. 261 (1996) 155
Baerends, E.J., V. Branchadell and M. Sodupe, Atomic reference energies for density functional calculations 265 (1997) 481
Bagryanskaya, E.G., V.R. Gorelik and R.Z. Sagdeev, Switched external magnetic field (SEMF) CIDNP – a new technique for investigation of the spin dynamics and kinetics of short-lived reaction intermediates in weak magnetic fields 264 (1997) 655
Bahou, M., L. Schriver-Mazzuoli, C. Camy-Peyret, A. Schriver, T. Chiavassa and J.P. Aycard, Infrared matrix spectra of the $N_2O \cdots O_2$ complex in solid nitrogen. The $N_2O \cdots O_2 + O$ thermal diffusion limited reaction 265 (1997) 145
Bai, Y., see Ravichandran, K. 261 (1996) 261
Bai, Y., see Volkmer, A. 268 (1997) 439
Bailey, C.G. and M.A. Johnson, Determination of the relative photodetachment cross sections of the two isomers of $(H_2O)_6^-$ using saturated photodetachment 265 (1997) 185
Bailey, C.G., J. Kim, C.E.H. Dessent and M.A. Johnson, Vibrational predissociation spectra of $I^- \cdot (H_2O)$: isotopic labels and weakly bound complexes with Ar and N_2 269 (1997) 122
Bailey, C.G., see Tsukuda, T. 269 (1997) 17
Bailey, J., see Grannan, S.M. 264 (1997) 359
Balakrishnan, G. and S. Umapathy, Intermolecular hydrogen atom abstraction from the fluoranil triplet excited state: a Raman study 270 (1997) 557
Balasubramanian, K. and D. Dai, Electronic states and potential energy surfaces of the tungsten trimer (W_3) 265 (1997) 538
Balasubramanian, K. and H. Sun, Euclidean inverses for the characterization of three-dimensional molecular structures 264 (1997) 70
Balasubramanian, K., see Dai, D. 263 (1996) 703
Balasubramanian, K., see Feng, P.Y. 265 (1997) 547
Balasubramanian, K., see Feng, P.Y. 265 (1997) 41
Balasubramanian, K., see Latifzadeh-Masoudipour, L. 262 (1996) 553
Balasubramanian, K., see Latifzadeh-Masoudipour, L. 267 (1997) 545
Balasubramanian, K., see Majumdar, D. 262 (1996) 263
Balasubramanian, K., see Roszak, S. 265 (1997) 553
Balasubramanian, K., see Feng, P.Y. 264 (1997) 449
Balasubramanian, K., see Roszak, S. 264 (1997) 80
Ball, G.E., G.J. Bowden, T.H. Heseltine, M.J. Prandolini and W. Bermel, Radiation damping artifacts in 2D COSY NMR experiments 261 (1996) 421
Ball, S.M., G. Hancock, S.E. Martin and J.C. Pinot de Moira, A direct measurement of the $O(^1D)$ quantum yields from the photodissociation of ozone between 300 and 328 nm 264 (1997) 531
Ballenweg, S., see Gromov, A. 267 (1997) 460
Baltuška, A., I.H.M. van Stokkum, A. Kroon, R. Monshouwer, K.J. Hellingwerf and R. van Grondelle, The primary events in the photoactivation of yellow protein 270 (1997) 263
Bal'zhinimaev, B.S., see Resnyanskii, E.D. 264 (1997) 174
Bañares, L., T. Baumert, M. Bergt, B. Kiefer and G. Gerber, Femtosecond photodissociation dynamics of $Fe(CO)_5$ in the gas phase 267 (1997) 141
Bañares, L., see Aoiz, F.J. 262 (1996) 175
Bañares, L., see Wrede, E. 265 (1997) 129
Bandyopadhyay, P., see Chaudhury, P. 262 (1996) 764
Banhart, F., T. Füller, Ph. Redlich and P.M. Ajayan, The formation, annealing and self-compression of carbon onions under electron irradiation 269 (1997) 349

Bar, I., see Arusi-Parpar, T. 268 (1997) 163
Baraldi, A., see Comelli, G. 261 (1996) 253
Baranov, L.Ya., see Held, A. 267 (1997) 318
Barbarotto, A., see Borghesani, A.F. 267 (1997) 116
Barborini, E., see Biasioli, F. 270 (1997) 115
Bardeen, C.J., see Cerullo, G. 262 (1996) 362
Barford, W. and R.J. Bursill, Theory of molecular excitons in the phenyl-based organic semiconductors 268 (1997) 535
Barigelletti, F., see Ghedini, M. 267 (1997) 341
Barnes, I., see Wängberg, I. 261 (1996) 138
Barnes, P.W., see Reid, J.P. 268 (1997) 150
Barone, V., Electronic, vibrational and environmental effects on the hyperfine coupling constants of nitroside radicals. H_2NO as a case study 262 (1996) 201
Barone, V., see Adamo, C. 263 (1996) 113
Baroni, S., see Lorentzen, J.D. 270 (1997) 129
Barrois, R., S. Bekavac and H. Kleindienst, Nonrelativistic energies for the lowest $^4P^o$ states of the Li isoelectronic series 268 (1997) 531
Barth, J.V., T. Zambelli, J. Wintterlin and G. Ertl, Hot precursors in the adsorption of molecular oxygen on Ag(110) 270 (1997) 152
Bartlett, R.J., see Gutsev, G.L. 265 (1997) 12
Bartlett, R.J., see Nooijen, M. 266 (1997) 456
Baskar, G. and A.B. Mandal, Molecular dynamics of methoxy polyoxyethylene macromonomer micelles in the absence and presence of SDS micelles using ^1H NMR spin–lattice relaxation time measurements 266 (1997) 443
Basko, D.M., see Argyrakis, P. 268 (1997) 372
Bässler, M., see Gebauer, W. 266 (1997) 177
Batirev, I.G., K.H. Lee, W.R. Lee, H.M. Lee and J.A. Leiro, Full-potential linear muffin-tin orbital calculation of atomic forces and optimization of atomic structure of fullerene epoxide derivatives $C_{60}O$ and $C_{60}O_2$ 262 (1996) 247
Bauer-Gogonea, S., W. Wirges, S. Bauer, R. Gerhard-Multhaupt, J. Liang and J. Zyss, Electrical determination of the degree of cross-linking in a poled non-linear optical polymer 262 (1996) 663
Bauer, S., see Bauer-Gogonea, S. 262 (1996) 663
Bauernschmitt, R., M. Häser, O. Treutler and R. Ahlrichs, Calculation of excitation energies within time-dependent density functional theory using auxiliary basis set expansions 264 (1996) 573
Baughman, R.H., D.S. Galvão, C. Cui and S.O. Dantas, Hinged and chiral polydiacetylene carbon crystals 269 (1997) 356
Baumert, T., see Bañares, L. 267 (1997) 141
Baumfalk, R., U. Buck, C. Frischkorn, S.R. Gandhi and C. Lauenstein, UV photolysis of $(HBr)_n$ clusters with known size distribution 269 (1997) 321
Baumgarten, M., L. Gherghel and T. Wehrmeister, Novel high-spin states in reduced dibenzoylbenzenes 267 (1997) 175
Baumgarten, M., see Zhang, J. 269 (1997) 187
Bauschlicher Jr., C.W., The $B(H_2)_n$–H_2 binding energies, for $n = 0$–3 261 (1996) 637
Bawagan, A.D.O. and E.R. Davidson, The potential energy surfaces of He_2^+: implications for femtosecond spectroscopy 266 (1997) 499
Beaud, P., see Radi, P.P. 265 (1997) 271

Becker, K.H., see Wängberg, I. 261 (1996) 138
Bedjanian, Y., G. Le Bras and G. Poulet, Kinetic study of the Br + IO, I + BrO and Br + I_2 reactions. Heat of formation of the BrO radical 266 (1997) 233
Beeby, A. and S. Faulkner, Luminescence from neodymium(III) in solution 266 (1997) 116
Bekavac, S., see Barrois, R. 268 (1997) 531
BelBruno, J.J., Ab initio calculations of the ring-opened and ring-closed isomers of $C_2H_4O^{+\cdot}$: the need for high level electron correlation techniques 263 (1996) 84
BelBruno, J.J., Ab initio calculations of the structures and energies of gas phase isomeric C_3N_4 molecules 270 (1997) 99
Beljonne, D., see Cross, G.H. 268 (1997) 36
Bell, T.D.M., T.A. Smith, K.P. Ghiggino, M.G. Ranasinghe, M.J. Shephard and M.N. Paddon-Row, Long-lived photoinduced charge separation in a bridged C_{60}-porphyrin dyad 268 (1997) 223
Bellert, D., see Buthelezi, T. 262 (1996) 303
Bellert, D., see Hayes, T. 264 (1997) 220
Belsky, A.N., see Zhang, L. 268 (1997) 408
Belton, P.S., see Wang, Y.L. 268 (1997) 387
Belu-Marian, A., see Mishori, B. 264 (1997) 163
Ben-Nun, M., T.J. Martínez and R.D. Levine, Multiple traversals of a conical intersection: electronic quenching in $Na^* + H_2$ 270 (1997) 319
Ben-Nun, M., T.J. Martínez, P.M. Weber and K.R. Wilson, Direct imaging of excited electronic states using diffraction techniques: theoretical considerations 262 (1996) 405
Benderskii, V.A., see Goldschleger, A.U. 267 (1997) 288
Bent, S.F., see Kong, M.J. 263 (1996) 1
Berardi, R., S. Orlandi and C. Zannoni, Antiphase structures in polar smectic liquid crystals and their molecular origin 261 (1996) 357
Berberan-Santos, M.N., see Fedorov, A. 267 (1997) 467
Berden, G., T. Groot, T. van der Veldt and G. Meijer, Doppler-free two-photon spectroscopy on the $S_1 \leftarrow S_0$ origin band of 1,4-diazabicyclo[2,2,2]octane (DABCO) 265 (1997) 204
Berden, G., see Engeln, R. 262 (1996) 105
Berden, G., see Jongma, R.T. 270 (1997) 304
Berg, C., see Albert, G. 268 (1997) 235
Bergt, M., see Bañares, L. 267 (1997) 141
Berkowitz, M.L., see Yeh, I.-C. 264 (1997) 31
Berlin, Yu.A. and A.L. Burin, Hierarchically constrained dynamics of the configurational coordinate for rate processes in complex systems 267 (1997) 234
Berlin, Yu.A., see Siebbeles, L.D.A. 265 (1997) 460
Bermel, W., see Ball, G.E. 261 (1996) 421
Bernath, P.F., see Colarusso, P. 269 (1997) 39
Berry, A.J., R.G. Denning and I.D. Morrison, Two-photon excitation spectroscopy of lanthanide elpasolites – implications for the correlation crystal field 266 (1997) 195
Berry, R.J., C.J. Ehlers, D.R. Burgess Jr., M.R. Zachariah and P. Marshall, A computational study of the reactions of atomic hydrogen with fluoromethanes: kinetics and product channels 269 (1997) 107
Berry, R.J., see Marshall, P. 265 (1997) 48
Bertault, M., see Even, J. 267 (1997) 585
Bertini, I., C. Luchinat and A. Rosato, Evaluation of paramagnetic relaxation rates in a *J*-coupled two-spin system (Chem. Phys. Letters 250 (1996) 495). Erratum 265 (1997) 677

Bertolotti, S.G., see Rivarola, C. 262 (1996) 131
Besnard, M., see Cabaco, M.I. 262 (1996) 120
Besnard, M., see Tassaing, T. 267 (1997) 496
Bessho, K., T. Uchida, A. Yamauchi, T. Shioya and N. Teramae, Microenvironments of 8-anilino-1-naphthalenesulfonate at the heptane–water interface: time-resolved total internal reflection fluorescence spectroscopy 264 (1997) 381
Bethune, D.S., see Grannan, S.M. 264 (1997) 359
Beutler, A., see Andersen, J.N. 269 (1997) 371
Bevan, J.W., see Han, J. 265 (1997) 209
Bevan, J.W., see Han, J. 264 (1997) 411
Beyer, M., see Albert, G. 268 (1997) 235
Bezrukov, O.F., see Veracini, C.A. 263 (1996) 228
Bhattacharyya, S., L.R. Sousa and S. Ghosh, Dual phosphorescence from 2,3-naphtho-17-crown-5 ether in ethanol glass at 77 K 269 (1997) 314
Bhattacharyya, S.P., see Adhikari, S. 265 (1997) 99
Bhattacharyya, S.P., see Chaudhury, P. 262 (1996) 764
Biasioli, F., A. Boschetti, E. Barborini, P. Piseri, P. Milani and S. Iannotta, Photofragmentation of C_{60} in seeded supersonic molecular beams: effects of ro-vibrational cooling 270 (1997) 115
Biemans, T., see Hendrickx, E. 270 (1997) 241
Bieniek, R.J. and S.J. Lipson, Semiquantal modeling of thermal vibrational relaxation of diatomic molecules 263 (1996) 276
Biesheuvel, C.A., D.H.A. ter Steege, J. Bulthuis, M.H.M. Janssen, J.G. Snijders and S. Stolte, High-resolution bolometric spectroscopy of NO_2 in the region of 13352 cm^{-1} 269 (1997) 515
Bieske, E.J., see Meuwly, M. 270 (1997) 252
Bieske, E.J., see Nizkorodov, S.A. 265 (1997) 303
Biglino, D., see Li, H. 266 (1997) 417
Bingham, S.J., D. Suter, A. Schweiger and A.J. Thomson, Optical detection of transition metal ion electron paramagnetic resonance by coherent Raman spectroscopy 266 (1997) 543
Binnemans, K., K. Van Herck and C. Görller-Walrand, Influence of dipicolinate ligands on the spectroscopic properties of europium(III) in solution 266 (1997) 297
Birch, D.J.S., see Holmes, A.S. 266 (1997) 309
Birch, D.J.S., see Lopez, M. 268 (1997) 125
Birch, D.J.S., see Volkmer, A. 268 (1997) 439
Birmingham, J.T., see Grannan, S.M. 264 (1997) 359
Biswas, R., B. Nath and C. Sinha, Triple differential cross sections for electron impact ionisation of alkali like ion Mg^+ 263 (1996) 495
Biswas, R., B. Nath and C. Sinha, Triple differential cross sections for electron impact ionisation of alkali like ion Mg^+ (Chem. Phys. Letters 263 (1996) 495). Erratum 269 (1997) 186
Bittl, R., see Zweygart, W. 261 (1996) 272
Bitto, H. and R.T. Carter, Comment on ''Lifetimes of vibrational levels in the $\tilde{B}\ ^2A'$ state of HCO'' 261 (1996) 385
Bitto, H. and S. Gfeller, The S_1 dynamics of 4- and 5-methylpyrimidine: the role of frame and internal rotor symmetries 265 (1997) 600
Bitto, H., see Gejo, T. 261 (1996) 443
Bizzarri, A.R., C. Rocchi and S. Cannistraro, Origin of the anomalous diffusion observed by MD simulation at the protein–water interface 263 (1996) 559
Blackford, M., see Gadd, G.E. 261 (1996) 221
Blackford, M., see Gadd, G.E. 270 (1997) 108

Blaisten-Barojas, E., see Li, Y. 268 (1997) 331
Blake, G.A., see Rodham, D.A. 264 (1997) 522
Blau, W.J., see Henari, F.Z. 267 (1997) 229
Blaudeau, J.P., see Deutsch, P.W. 270 (1997) 413
Bloor, D., see Cross, G.H. 268 (1997) 36
Bludau, H., see Schwegmann, S. 264 (1997) 680
Blumstengel, S., see Frankevich, E.L. 261 (1996) 545
Bobbio, T.B., see Jorge, F.E. 263 (1996) 775
Bodenhausen, G., see Fu, R. 264 (1997) 63
Boens, N., see Molski, A. 266 (1997) 139
Boeré, R.T., see Moazzen-Ahmadi, N. 265 (1997) 563
Boero, M. and W. Andreoni, Trimethylene isomers and propene: structural and vibrational properties from density functional theory 265 (1997) 24
Bofill, J.M., see Anglada, J.M. 269 (1997) 469
Bogart, K.H.A., J.P. Cushing and E.R. Fisher, Surface reactivity measurements for OH radicals during deposition of SiO_2 from tetraethoxysilane/O_2 plasmas 267 (1997) 377
Bohr, F., see Henon, E. 264 (1997) 557
Boissoles, J., see Khalil, B. 263 (1996) 811
Boldyrev, A.I. and J. Simons, Predictions of ground states of LiGa and NaGa 262 (1996) 807
Bondybey, V.E., see Albert, G. 268 (1997) 235
Bonechi, C., see Rossi, C. 264 (1997) 205
Bonetti, G., A. Vecli and C. Viappiani, Reaction volume of water formation detected by time-resolved photoacoustics: photoinduced proton transfer between *o*-nitrobenzaldehyde and hydroxyls in water 269 (1997) 268
Bongiorno, A., L. Colombo and F. Cargnoni, Hydrogen diffusion in crystalline SiO_2 264 (1997) 435
Booij, A.S., see Kovács, A. 268 (1997) 207
Booth, J.P., see Cunge, G. 263 (1996) 645
Bopp, M.A., A.J. Meixner, G. Tarrach, I. Zschokke-Gränacher and L. Novotny, Direct imaging single molecule diffusion in a solid polymer host 263 (1996) 721
Borbat, P., see Raitsimring, A. 262 (1996) 8
Bordiga, S., see Lamberti, C. 269 (1997) 500
Borghesani, A.F., D. Neri and A. Barbarotto, Mobility of O_2^- ions in near critical Ar gas 267 (1997) 116
Borin, A.C., A complete active space self-consistent field and multireference configuration interaction analysis of the SiN B $^2\Sigma^+ - X\ ^2\Sigma^+$ transition moment 262 (1996) 80
Borovkov, V.I., S.V. Anishchik and O.A. Anisimov, Time-resolved electric field effects in recombination fluorescence as a method of studying primary radiation–chemical processes 270 (1997) 327
Borsarelli, C.D., see Rivarola, C. 262 (1996) 131
Børve, K.J., On the calculation of molecular field splitting in S 2p photoelectron spectra 262 (1996) 801
Boschetti, A., see Biasioli, F. 270 (1997) 115
Bosi, L., D. Gallo and M. Zelada, On the lifetime of KCl:Ag^+ fluorescence 267 (1997) 123
Bouanich, J.P., see Ozanne, L. 261 (1996) 353
Boulet, C., see Ozanne, L. 261 (1996) 353
Bouř, P., Approximate ab initio calculations of polarizabilities via the excitation scheme 265 (1997) 65
Bourcier, W.L., see Wilson, W.D. 267 (1997) 431
Boutton, C., see Hendrickx, E. 270 (1997) 241
Bowden, G.J., see Ball, G.E. 261 (1996) 421
Bowen, K.H., see Tsukuda, T. 269 (1997) 17

Bowman, J.M., see Dzegilenko, F.N. 264 (1997) 24
Bozio, R., see Mulloni, V. 263 (1996) 331
Bozzelli, J.W., see Lay, T.H. 268 (1997) 175
Bradley, D.D.C., see Lidzey, D.G. 263 (1996) 655
Bramley, R., see Delfs, C.D. 264 (1997) 333
Branca, M., see Rustici, M. 263 (1996) 429
Branchadell, V., see Baerends, E.J. 265 (1997) 481
Bratos, S. and J.-.C. Leicknam, Ultrafast transient absorption spectroscopy of the hydrated electron: a theory 261 (1996) 117
Braun, D. and W. Rettig, Excitation energy dependence of the kinetics of charge-transfer formation 268 (1997) 110
Braun, E., O.L. Fuchs and S. Godoy, Hydrodynamic mobilities in a suspension with a fluid with spin 265 (1997) 434
Brédas, J.-L., see Cross, G.H. 268 (1997) 36
Breidung, J., W. Thiel and J. Demaison, Equilibrium structure of PH_2Br 266 (1997) 515
Bremi, T., see Straus, S.K. 262 (1996) 709
Brena, B., see Polzonetti, G. 267 (1997) 384
Bressler, C.G., see Dyer, M.J. 266 (1997) 548
Bretón, J., see Ruiz, A. 270 (1997) 121
Breton, J., see Iglesias-Groth, S. 264 (1997) 351
Brezina, R., S.H. Lin and W.-K. Liu, Quantum mechanical calculation of line shape parameters for the depolarized Raman Q branch of D_2 in He 262 (1996) 437
Brezová, V., see Staško, A. 262 (1996) 233
Brint, R.P., see Ruth, A.A. 264 (1997) 605
Brion, J., see Henon, E. 264 (1997) 557
Britt, B.M. and J.L. McHale, Resonance Raman study of a two-chromophore system. The 2:1 complex of hexamethylbenzene with tetracyanoethylene 270 (1997) 551
Brivio, G.P., M.L. Rossi and T.B. Grimley, Results for dissociative sticking from a parametrization of an exactly solvable model 263 (1996) 597
Bródka, A., see Gwóźdź, E. 267 (1997) 557
Brodsky, A., Is there predictive value in water computer simulations? 261 (1996) 563
Brouard, M., see Alexander, A.J. 262 (1996) 589
Brouard, M., see Aoiz, F.J. 264 (1997) 487
Brownsword, R.A., M. Hillenkamp, T. Laurent, R.K. Vatsa, H.-R. Volpp and J. Wolfrum, Quantum yield for H atom formation in the methane dissociation after photoexcitation at the Lyman-α (121.6 nm) wavelength 266 (1997) 259
Broyer, M., see Antoine, R. 261 (1996) 670
Brucat, P.J., see Buthelezi, T. 262 (1996) 303
Brucat, P.J., see Hayes, T. 264 (1997) 220
Brugh, D.J. and M.D. Morse, Resonant two-photon ionization spectroscopy of the 13-electron triatomic Si_2N 267 (1997) 370
Brumer, P., see Dods, J. 261 (1996) 612
Brummel, C.L., see Willey, K.F. 267 (1997) 359
Brunold, T.C., H.U. Güdel and E. Cavalli, Optical spectroscopy of Ni^{2+} doped crystals of Zn_2SiO_4 268 (1997) 413
Brüschweiler, R., Nuclear spin relaxation and non-ergodic quasi-equilibria 270 (1997) 217
Brüschweiler, R. and R.R. Ernst, Non-ergodic quasi-equilibria in short linear spin 1/2 chains 264 (1997) 393

Brüschweiler, R., see Mádi, Z.L. 268 (1997) 300
Brutscher, B., see Mádi, Z.L. 268 (1997) 300
Buatier de Mongeot, F., A. Cupolillo, U. Valbusa and M. Rocca, O_2 dissociation on Ag(001): the role of kink sites 270 (1997) 345
Buatier de Mongeot, F., see Åkerlund, C. 270 (1997) 157
Buchachenko, A.A. and N.F. Stepanov, Structure and interaction energies of the Ar...Cl_2 complex. Application of first-order intermolecular potentials 261 (1996) 591
Buchachenko, A.A., T. Gonzalez-Lezana, M.I. Hernandez, G. Delgado-Barrio, P. Villarreal and N.F. Stepanov, Half- and full-collision VT energy transfer in the He–Br_2(B) system 269 (1997) 448
Bucher, G., see Kraka, E. 268 (1997) 313
Buck, U., see Baumfalk, R. 269 (1997) 321
Buckingham, A.D., see Read, J.P. 270 (1997) 245
Buenker, R.J., see Wright, J.S. 266 (1997) 391
Bueno, M.I., see Kubota, L.T. 264 (1997) 662
Bühl, M., Density functional computations of transition metal NMR chemical shifts: dramatic effects of Hartree–Fock exchange 267 (1997) 251
Bukowska, J., A. Kudelski and M. Janik-Czachor, SERS on modified amorphous Cu–Zr alloys 268 (1997) 481
Bukowski, R., see Williams, H.L. 262 (1996) 431
Bulthuis, J., see Biesheuvel, C.A. 269 (1997) 515
Bündgen, P., A.J. Thakkar, F. Grein, M. Ernzerhof, C.M. Marian and B. Nestmann, Moments of the quadrupole oscillator strength distribution for O_2, N_2, CO, HF, HCl, N_2O, CO_2, OCS, CS_2 and C_2H_2: ab initio sum rule calculations 261 (1996) 625
Buntkowsky, G., see Dvinskikh, S.V. 268 (1997) 401
Burak, I., see Alexander, A.J. 262 (1996) 589
Burbank, P., see Grannan, S.M. 264 (1997) 359
Bureau, C. and D.P. Chong, Density functional calculations of core-electron binding energies of amines. Application to $(CH_3)_3N$–Ni and $(CH_3)_4N^+$–Ni 264 (1997) 186
Bureau, C., A DFT-based procedure for predicting core-electron binding energies of chemisorbed molecules using small cluster models: first tests on CO on Ni(100), Pd(100) and Pd(110) 269 (1997) 378
Bürger, H., H. Ruland and L. Fusina, Ground state rotational and $K = 3$ splitting parameters determined from high resolution infrared spectra: H $^{28}SiD_3$, H $^{70}GeD_3$ and H $^{120}SnD_3$ 268 (1997) 249
Burgess Jr., D.R., see Berry, R.J. 269 (1997) 107
Bürgi, T., see Wickleder, C. 264 (1997) 257
Burin, A.L., see Berlin, Yu.A. 267 (1997) 234
Bürk, M., see Cummins, T.R. 261 (1996) 228
Burke, K., M. Ernzerhof and J.P. Perdew, The adiabatic connection method: a non-empirical hybrid 265 (1997) 115
Burkholder, J.B., see Talukdar, R.K. 262 (1996) 669
Burshtein, A.I. and P.A. Frantsuzov, Photogeneration of ions and radicals in non-polar solutions 263 (1996) 513
Bursill, R.J., see Barford, W. 268 (1997) 535
Burton, N.A., see Akhmatskaya, E.V. 267 (1997) 105
Burton, N.A., see Andrews, S.B. 261 (1996) 521
Burton, N.A., see Andrews, S.B. 269 (1997) 475
Buthelezi, T., D. Bellert, T. Hayes and P.J. Brucat, The adiabatic binding energy of $NbAr^+$ 262 (1996) 303

Buthelezi, T., see Hayes, T. 264 (1997) 220
Butkovskaya, N.I., A.A. Muravyov and D.W. Setser, Infrared chemiluminescence from the NO + HCO reaction: observation of the $2\nu_1-\nu_1$ hot band of HNO 266 (1997) 223
Buttet, J., see Reuse, F.A. 267 (1997) 258
Byrom, P.G., see Spackman, M.A. 267 (1997) 215

Cabaco, M.I., Y. Danten, M. Besnard, Y. Guissani and B. Guillot, Evidence of dimer formation in neat liquid 1,3,5-trifluorobenzene 262 (1996) 120
Caballol, R., see García, V.M. 261 (1996) 98
Caballol, R., see Reguero, M. 265 (1997) 621
Cai, R., see Zhao, L. 263 (1996) 235
Cai, S.M., see Zhu, T. 265 (1997) 334
Calfas, R.S. and D.E. Weeks, A new application of absorbing boundary conditions for computing collinear quantum reactive scattering matrix elements 263 (1996) 292
Calhoun, A., M. Pavese and G.A. Voth, Hyper-parallel algorithms for centroid molecular dynamics: application to liquid para-hydrogen 262 (1996) 415
Callis, P.R., see Fender, B. 262 (1996) 343
Calogero, G., see Ghedini, M. 267 (1997) 341
Camaioni, N., see Kalinowski, J. 265 (1997) 607
Caminati, W., G. Maccaferri, P.G. Favero and L.B. Favero, Free jet absorption millimeter wave spectrum of purine (Chem. Phys. Lett. 251 (1996) 189). Erratum 265 (1997) 561
Caminati, W., P.G. Favero, S. Melandri and R. Meyer, Free jet absorption millimeter wave spectrum of the pyrimidine–argon molecular complex 268 (1997) 393
Caminati, W., see Melandri, S. 261 (1996) 267
Camy-Peyret, C., see Bahou, M. 265 (1997) 145
Candori, R., see de Castro Vítores, M. 263 (1996) 456
Canet, D., P. Mutzenhardt and F. Guenneau, Nuclear spin coherence transfer induced by a single static field gradient pulse 264 (1996) 477
Cannistraro, S., see Bizzarri, A.R. 263 (1996) 559
Canuto, S., see Serrano, A. 269 (1997) 193
Cao, J. and G.A. Voth, A theory for the quantum activated rate constant in dissipative systems 261 (1996) 111
Cao, Q., see Li, F. 264 (1997) 376
Cao, X., see Fischer, G. 262 (1996) 689
Capitelli, M., D. Giordano, C. Gorse and S. Longo, Effects of non-Boltzmann vibrational distributions on electron–molecule and bimolecular reaction rates 263 (1996) 635
Capitelli, M., see Dyatko, N.A. 263 (1996) 305
Caravati, C., see Rustici, M. 263 (1996) 429
Cárdenas, A.E. and R.D. Coalson, A wavepacket – path integral method for curve-crossing problems: application to resonance Raman spectra and photodissociation cross sections 265 (1997) 71
Cargnoni, F., see Bongiorno, A. 264 (1997) 435
Carlos, L.D. and A.L.L. Videira, Ion-chain effective field in polymer electrolytes 264 (1997) 57
Carlos del Valle, J., M. Kasha and J. Catalán, Chemical physics of excitation dynamics via amplified spontaneous emission (ASE) laser spike spectroscopy in substituted phenylox-azoles 263 (1996) 154
Carpenter, D.J., see Wright, J.S. 266 (1997) 391
Carrington, A., D.I. Gammie, A.M. Shaw and S.M. Taylor, Observation of a microwave spectrum of the long-range $He\cdots N^+$ complex 262 (1996) 598

Carrington, T., see Eng, R. 261 (1996) 651
Carrington Jr., T., see Miller, S.M. 267 (1997) 417
Carter, E.A., see Reynolds, G. 265 (1997) 660
Carter, R.T., see Bitto, H. 261 (1996) 385
Cassidy, D., see Gadd, G.E. 270 (1997) 108
Castaño, F., see Fernández, J.A. 267 (1997) 301
Castaño, O., see Notario, R. 263 (1996) 367
Castellano, E., see Cobos, C.J. 266 (1997) 253
Castillejo, M., M. Martín, R. de Nalda and J. Solís, Nanosecond versus picosecond near UV multiphoton dissociation of ketene 268 (1997) 465
Castillejo, M., see Martin, M. 266 (1997) 111
Castro, M., see Pápai, I. 267 (1997) 551
Catalán, J., J. Palomar and J.L.G. De Paz, Double- or single-well potential for GSIPT in 1-hydroxy-2-acetonaphthone? 269 (1997) 151
Catalán, J., see Carlos del Valle, J. 263 (1996) 154
Cavalleri, O., S.E. Gilbert and K. Kern, Growth manipulation in electrodeposition with self-assembled monolayers 269 (1997) 479
Cavalli, E., see Brunold, T.C. 268 (1997) 413
Cavell, R.G., see Kosugi, N. 265 (1997) 490
Celiberto, R., see Dyatko, N.A. 263 (1996) 305
Cencek, W. and W. Kutzelnigg, Accurate adiabatic correction for the hydrogen molecule using the Born–Handy formula 266 (1997) 383
Céolin, R., see Agafonov, V. 267 (1997) 193
Cerullo, G., C.J. Bardeen, Q. Wang and C.V. Shank, High-power femtosecond chirped pulse excitation of molecules in solution 262 (1996) 362
Ceursters, B., see Devriendt, K. 261 (1996) 450
Chaban, A.N., see Frankevich, E.L. 261 (1996) 545
Chabrier, P., see Del Bene, J.E. 264 (1997) 109
Chachisvilis, M. and V. Sundström, Femtosecond vibrational dynamics and relaxation in the core light-harvesting complex of photosynthetic purple bacteria 261 (1996) 165
Chakir, A., see Henon, E. 264 (1997) 557
Chakrabarti, N., C. Kalyanaraman and N. Sathyamurthy, Resonance de-enhancement in the continuum Raman spectrum of HI 267 (1997) 31
Chakravarti, N. and K.L. Sebastian, Fractional Brownian motion models for polymers 267 (1997) 9
Chambaud, G., see Robbe, J.M. 267 (1997) 91
Chambers, S.A., S. Thevuthasan, Y.J. Kim, G.S. Herman, Z. Wang, E. Tober, R. Ynzunza, J. Morais, C.H.F. Peden, K. Ferris and C.S. Fadley, Chemisorption geometry of formate on $TiO_2(110)$ by photoelectron diffraction 267 (1997) 51
Champagne, B., Vibrational polarizability and hyperpolarizability of *p*-nitroaniline 261 (1996) 57
Chan, C.M.-T., H. Li and A.S.-C. Cheung, Laser induced fluorescence spectroscopy of ZrN: rotational structure in the $A^2\Pi$–$X\,^2\Sigma$ (2,2) band 269 (1997) 49
Chan, K.-C., see Weng, Y.-X. 270 (1997) 315
Chance, M., see Haran, G. 261 (1996) 389
Chandra, A.K. and V. Sreedhara Rao, Two-dimensional tunneling of hydrogen in a Norrish type II process of a ketone 270 (1997) 87
Chandra, A.K. and M.T. Nguyen, Theoretical studies on the $H_2O \cdots ClF$ complex 268 (1997) 321
Chang, T.-M. and L.X. Dang, Transfer of CH_4 across the H_2O–CCl_4 liquid–liquid interface with polarizable potential models 263 (1996) 39

Chaquin, P., see Moulin, V. 263 (1996) 423
Charutz, D.M., R. Baer and M. Baer, A study of degenerate vibronic coupling effects on scattering processes: are resonances affected by degenerate vibronic coupling? 265 (1997) 629
Charutz, D.M., see Rom, N. 270 (1997) 382
Chattopadhyay, N., J. Rommens, M. Van der Auweraer and F.C. De Schryver, Laser-induced optoacoustic studies of the non-radiative deactivation of ICT probes DMABN and DMABA 264 (1997) 265
Chaudhury, P., P. Bandyopadhyay and S.P. Bhattacharyya, Exploring a discretized generator coordinate route to approximate eigenstates of one- and two-dimensional anharmonic oscillators within the framework of the simulated annealing method 262 (1996) 764
Che, C.-M., see Weng, Y.-X. 270 (1997) 315
Chen, G., see Lin, L.-R. 266 (1997) 358
Chen, G.-Z., see Du, X.-Z. 268 (1997) 31
Chen, J.-T., see Cheng, W.-D. 261 (1996) 66
Chen, L.X. and P.D. Laible, Third order nonlinear optical properties of bacteriochlorophylls in bacterial photosynthetic light-harvesting proteins 270 (1997) 255
Chen, M.C., see Liou, H.T. 266 (1997) 591
Chen, R. and H. Guo, Extraction of resonances via wave packet propagation in Chebyshev order domain: collinear $H + H_2$ scattering 261 (1996) 605
Chen, Y., see Zhao, L. 263 (1996) 235
Chen, Y., see Guo, L.P. 268 (1997) 26
Chen, Y., see Moler, E.J. 264 (1997) 502
Cheng, C.-F., W. Zhou and J. Klinowski, Directing the pore dimensions in the mesoporous molecular sieve MCM-41 263 (1996) 247
Cheng, C.-F., see Lee, M.-H. 265 (1997) 673
Cheng, G., see Gu, G. 270 (1997) 135
Cheng, W.-D., J.-T. Chen, J.-S. Huang and Q.-E. Zhang, Theoretical studies of the electronic structures and linear, nonlinear optics of $K_{3-x}Li_{2+x}Nb_5O_{15}$ with $x = 0$ and $x = 1$ 261 (1996) 66
Cheng, X., see Qiu, F. 266 (1997) 153
Cheon, H.W., see Kim, Y. 264 (1997) 673
Chergui, M., see Sassara, A. 261 (1996) 213
Chernishev, Yu.A., see Aleinikov, N.N. 267 (1997) 155
Chernozatonskii, L.A., see Kukovitskii, E.F. 266 (1997) 323
Chernozatonskii, L.A., see Gal'pern, E.G. 269 (1997) 85
Cheung, A.S.-C., see Chan, C.M.-T. 269 (1997) 49
Chiavassa, T., see Bahou, M. 265 (1997) 145
Child, M.S., see Weston, T. 262 (1996) 751
Chin, W.S., see Huang, H.H. 265 (1997) 508
Chirvony, V.S., see Kruglik, S.G. 270 (1997) 293
Chistyakov, A.L., see Gal'pern, E.G. 269 (1997) 85
Chitra, K., see Subramanian, V. 264 (1997) 92
Cho, B.R., see Song, N.W. 261 (1996) 307
Choi, C.H. and M. Kertesz, A new partition of the atomic polar tensor: the benzene molecule 263 (1996) 697
Choi, H.S., see Kim, K.S. 265 (1997) 497
Choi, J., see McIlroy, D.N. 264 (1997) 168
Chong, D.P., see Hu, C.-H. 262 (1996) 729

Chong, D.P., see Hu, C.-H. 262 (1996) 733
Chong, D.P., see Bureau, C. 264 (1997) 186
Chosrowjan, H., N. Mataga, N. Nakashima, Y. Imamoto and F. Tokunaga, Femtosecond–picosecond fluorescence studies on excited state dynamics of photoactive yellow protein from *Ectothiorhodospira halophila* 270 (1997) 267
Christiansen, O., H. Koch, P. Jørgensen and T. Helgaker, Integral direct calculation of CC2 excitation energies: singlet excited states of benzene 263 (1996) 530
Christiansen, O., J. Gauss and J.F. Stanton, Nuclear magnetic shielding constants in the CC2 model 266 (1997) 53
Christiansen, O., J. Olsen, P. Jørgensen, H. Koch and P.-Å. Malmqvist, On the inherent divergence in the Møller–Plesset series. The neon atom – a test case 261 (1996) 369
Christiansen, O., see Hättig, C. 269 (1997) 428
Chu, S.-I, see Telnov, D.A. 264 (1997) 466
Chu, Z.T., see Warshel, A. 265 (1997) 293
Chudoba, C., E. Riedle, M. Pfeiffer and T. Elsaesser, Vibrational coherence in ultrafast excited state proton transfer 263 (1996) 622
Cicman, P., see Matejcik, S. 261 (1996) 437
Cicman, P., see Matejcik, S. 267 (1997) 329
Cihlář, A., see Rodová, M. 268 (1997) 455
Ciofalo, M. and G. La Manna, Ab initio conformational study of 2,2′:5′,2″-terthiophene 263 (1996) 73
Cirujeda, J., see Deumal, M. 265 (1997) 190
Cisse, O., see Khalil, B. 263 (1996) 811
Clary, D.C., see Munn, N.S. 266 (1997) 437
Clary, D.C., see Sorenson, J.M. 263 (1996) 680
Clary, D.C., see Wang, L. 262 (1996) 284
Clays, K., see Hendrickx, E. 270 (1997) 241
Coalson, R.D., see Cárdenas, A.E. 265 (1997) 71
Cobos, C.J., A.E. Croce and E. Castellano, Kinetics of the reaction of Cl atoms with FC(O)O and FC(O)OCl 266 (1997) 253
Cocco, D., see Comelli, G. 261 (1996) 253
Cocco, D., see Polzonetti, G. 267 (1997) 384
Cohen, H., see Haran, A. 268 (1997) 475
Colarusso, P., K.Q. Zhang, B. Guo and P.F. Bernath, The infrared spectra of uracil, thymine, and adenine in the gas phase 269 (1997) 39
Colbert, D.T., see Nikolaev, P. 266 (1997) 422
Colmenares, F., see Hernández-Trujillo, J. 265 (1997) 503
Colombo, L., see Bongiorno, A. 264 (1997) 435
Comay, E., Comment on the longitudinal magnetic field of circularly polarized electromagnetic waves 261 (1996) 601
Comelli, G., A. Baraldi, S. Lizzit, D. Cocco, G. Paolucci, R. Rosei and M. Kiskinova, Real-time X-ray photoelectron spectroscopy study of dissociative oxygen adsorption on Rh(110) 261 (1996) 253
Contreras, R., see Pérez, P. 269 (1997) 419
Conwell, E.M., see Wu, M.W. 266 (1997) 363
González Ureña, A., see de Castro Vítores, M. 263 (1996) 456
Cooke, S.A., G. Cotti, C.M. Evans, J.H. Holloway and A.C. Legon, Rotational spectrum and properties of a gas-phase complex of molecular fluorine and hydrogen cyanide 262 (1996) 308

Cooke, S.A., J.H. Holloway and A.C. Legon, The rotational spectrum and angular geometry of a pre-reactive complex of allene and chlorine monofluoride 266 (1997) 61
Coombes, D.S., G.K. Nagi and S.L. Price, On the lack of hydrogen bonds in the crystal structure of alloxan 265 (1997) 532
Cooper, M.D., see Akhmatskaya, E.V. 267 (1997) 105
Cooper, M.J. and C.M. Western, Two-colour double resonance multiphoton ionisation spectroscopy of S_2 267 (1997) 365
Copeland, R.A., see Dyer, M.J. 266 (1997) 548
Corbini, G., see Rossi, C. 264 (1997) 205
Corcelli, S.A. and J.D. Doll, A Bayesian approach to short-time quantum dynamics: quantum instantaneous normal modes 263 (1996) 671
Corma, A., see Sastre, G. 264 (1997) 565
Corti, P., see Rossi, C. 264 (1997) 205
Cosa, J.J., see Rivarola, C. 262 (1996) 131
Costas, M., see Hernández-Trujillo, J. 265 (1997) 503
Costes, M., see Naulin, C. 266 (1997) 335
Cotti, G., C.M. Evans, J.H. Holloway and A.C. Legon, Rotational spectroscopy of a pre-reactive mixture of H_2S and F_2: detection and characterisation of the weakly bound complex $H_2S \cdots F_2$ 264 (1997) 513
Cotti, G., see Cooke, S.A. 262 (1996) 308
Cowen, K.A., see Lorenz, K.T. 261 (1996) 145
Cowley, J.M., P. Nikolaev, A. Thess and R.E. Smalley, Electron nano-diffraction study of carbon single-walled nanotube ropes 265 (1997) 379
Cremer, D., see Kraka, E. 268 (1997) 313
Croce, A.E., see Cobos, C.J. 266 (1997) 253
Cross, G.H., D. Healy, M. Szablewski, D. Bloor, M. Malagoli, T. Kogej, D. Beljonne and J.-L. Brédas, Highly polar chromophores in poled polymer films characterised by second harmonic generation 268 (1997) 36
Cross, R.J., see Curotto, E. 269 (1997) 183
Cue, N., see Ding, J. 261 (1996) 92
Cuevas, G., see Hernández-Trujillo, J. 265 (1997) 503
Cui, C., see Baughman, R.H. 269 (1997) 356
Cui, Q. and K. Morokuma, Ab initio MO studies on the photodissociation of the methoxy family CX_3Y (X = H, F; Y = O, S) from the $\tilde{A}\,^2A_1$ state 263 (1996) 54
Cui, Q., K. Morokuma and J.F. Stanton, Ab initio MO studies on the photodissociation of C_2H_2 from the S_1 (^1A_u) state. Non-adiabatic effects and S–T interaction 263 (1996) 46
Cummins, T.R., M. Bürk, M. Schmidt, J.F. Armbruster, D. Fuchs, P. Adelmann, S. Schuppler, R.H. Michel and M.M. Kappes, Electronic states and molecular symmetry of the higher fullerene C_{80} 261 (1996) 228
Cunge, G., J.P. Booth and J. Derouard, Absolute concentration measurements by pulsed laser-induced fluorescence in low-pressure gases: allowing for saturation effects 263 (1996) 645
Cupolillo, A., see Åkerlund, C. 270 (1997) 157
Cupolillo, A., see Buatier de Mongeot, F. 270 (1997) 345
Curotto, E. and R.J. Cross, The perturbation representation for molecular inelastic scattering 269 (1997) 183
Curtiss, L.A., K. Raghavachari, P.C. Redfern and J.A. Pople, Investigation of the use of B3LYP zero-point energies and geometries in the calculation of enthalpies of formation 270 (1997) 419
Curtiss, L.A., see Deutsch, P.W. 270 (1997) 413

Curtiss, L.A., see Sutjianto, A. 264 (1997) 127
Curtiss, T.J., see Hain, T.D. 262 (1996) 723
Cushing, J.P., see Bogart, K.H.A. 267 (1997) 377
Czapla, Z., see Ryba-Romanowski, W. 264 (1997) 323

Dabestani, R., see Rollins, H.W. 268 (1997) 187
Dabkara, N.K., see Agrawal, P.M. 266 (1997) 481
D'Acapito, F., see Lamberti, C. 269 (1997) 500
Dai, D. and K. Balasubramanian, Electronic states of Rh_4 263 (1996) 703
Dai, D., see Balasubramanian, K. 265 (1997) 538
Dai, H.-L., see Xue, B. 265 (1997) 154
Dai, S., W. Xu, D.H. Metcalf and L.M. Toth, Energy transfer between UO_2^{2+} and Eu^{3+} in sol–gel glasses: a spectroscopic investigation 262 (1996) 315
Dang, L.X., see Chang, T.-M. 263 (1996) 39
Daniel, H., see Yamazaki, T. 265 (1997) 137
Dantas, S.O., see Baughman, R.H. 269 (1997) 356
Danten, Y., see Cabaco, M.I. 262 (1996) 120
Das, G.P., see Majumder, C. 261 (1996) 515
Da Silva, A.B.F., see Jorge, F.E. 263 (1996) 775
Daudey, J.P., see Romero, T. 261 (1996) 583
Daul, C., M. Frioud, O. Schafer and A. Selloni, Non-empirical dynamical DFT calculation of the Berry pseudorotation of PF_5 262 (1996) 74
Davidovich, R.L., see Gabuda, S.P. 263 (1996) 253
Davidson, E.R., see Bawagan, A.D.O. 266 (1997) 499
Davison, S.G., see Taferner, W.T. 269 (1997) 171
Davydov, V.A., see Agafonov, V. 267 (1997) 193
De Andrés, J., see Romero, T. 261 (1996) 583
De Castro Vítores, M., R. Candori, F. Pirani, V. Aquilanti, M. Garay and A. Conzález Ureña, Determination of D_0^0(Ca...HBr) from full and half collision studies. Van der Waals and charge transfer contributions to the formation of Ca...Hx (X = Cl, Br) complexes 263 (1996) 456
Deck, R.T., see Piryatinski, A. 269 (1997) 156
Decurtins, S., see Hauser, A. 261 (1996) 313
Dedonder-Lardeux, C., C. Jouvet, S. Martrenchard-Barra, D. Solgadi and I. Dimicoli, Ionic nucleophilic substitution in halobenzene–NH_3 complexes: the entrance channel 264 (1997) 596
Deeth, R.J., Transition state symmetries and theoretical activation enthalpies for chloride exchange at planar $[PdCl_4]^{2-}$ 261 (1996) 45
Dehe, K. and H. Heydtmann, HF infrared emission from the reactions of atomic fluorine with methylcyanide, methylisocyanide, dimethylsulfide and dimethyldisulfide 262 (1996) 683
Deimel, M., see Müller, R. 262 (1996) 716
Delaney, N., see Faeder, J. 270 (1997) 196
Del Barrio, J.I., R. Fernández Cézar and F.M. G-Tablas, Pulsed infrared carbon selective dissociation of CF_3Br with N_2 and D_2 as buffers 270 (1997) 71
Del Bene, J.E., K. Szczepaniak, P. Chabrier and W.B. Person, Ab initio theoretical and matrix isolation experimental studies of hydrogen bonding: evidence of a dramatic effect of the matrix on the structure and vibrational spectrum of HBr:3,5-dichloropyridine 264 (1997) 109
Del Buono, G.S., F.E. Figueirido and R.M. Levy, Dielectric response of solvent surrounding an ion pair: Ewald potential versus spherical truncation 263 (1996) 521

Delfs, C.D. and R. Bramley, The zero-field EPR spectrum of a copper dimer 264 (1997) 333
Delgado-Barrio, G., see Buchachenko, A.A. 269 (1997) 448
Deligiannakis, Y., C. Jegerschöld and A.W. Rutherford, EPR and ESEEM study of the plastoquinone anion radical $Q_A^{-\cdot}$ in photosystem II treated at high pH 270 (1997) 564
Delisle, C.J., see Roney, A. 270 (1997) 59
Della Védova, C.O., see Gobbato, K.I. 266 (1997) 527
Deltau, G., see Müller, R. 262 (1996) 716
Délugeard, Y., see Even, J. 267 (1997) 585
Demaison, J., see Breidung, J. 266 (1997) 515
De Melo, C.P. and T.L. Fonseca, Ab initio polarizabilities of polyenic chains with conformational defects 261 (1996) 28
Demmer, D.R.M., see Abou-Zied, O.K. 266 (1997) 75
Demtröder, W., see Färbert, A. 264 (1997) 225
De Nalda, R., see Castillejo, M. 268 (1997) 465
Deng, L., W.R. Garrett, M.G. Payne and M.A. Moore, Gain suppression involving both stimulated Raman and hyper-Raman photons in two-step stimulated emissions 270 (1997) 299
Deng, W.-Q., see Zhan, J.-P. 264 (1997) 687
Denning, R.G., see Berry, A.J. 266 (1997) 195
De Oliveira, G. and C.E. Dykstra, Quantum Monte Carlo study of the ground vibrational states of Ar_{2-6}–H_2S clusters. A case of microsolvation 264 (1997) 85
De Oliveira Neto, G., see Kubota, L.T. 264 (1997) 662
De Paz, J.L.G., see Catalán, J. 269 (1997) 151
De Proft, F. and P. Geerlings, Ab initio and density functional study of the Jahn–Teller distortion in the silane radical cation 262 (1996) 782
Der Chao, S., S.H. Lin, H.L. Selzle and E.W. Schlag, Comment on the spontaneous emission rates of ZEKE states 265 (1997) 445
Deren, P.J., J. Feries, J.-C. Krupa and W. Strek, Anti-Stokes emission in $LaCl_3$ doped with U^{3+} and Pr^{3+} ions 264 (1997) 614
Derouard, J., see Cunge, G. 263 (1996) 645
De Schryver, F.C., see Imans, F. 262 (1996) 583
De Schryver, F.C., see Chattopadhyay, N. 264 (1997) 265
Deshpande, A.V. and E.B. Namdas, Efficient lasing action of Rhodamine 6G in Nafion membranes 263 (1996) 449
De Silvestri, S., see Lanzani, G. 264 (1997) 667
De Souza, I.C.L., L.G. Mendes, M. Engelsberg and R.E. de Souza, Rotating frame proton spin–lattice relaxation in the glass transition region: a study of glycerol 264 (1996) 584
De Souza, R.E., see de Souza, I.C.L. 264 (1996) 584
Dessent, C.E.H., see Bailey, C.G. 269 (1997) 122
Dessent, C.E.H., see Tsukuda, T. 269 (1997) 17
Destombes, J.L., see Hadj Bachir, I. 270 (1997) 533
Deumal, M., J. Cirujeda, J. Veciana, M. Kinoshita, Y. Hosokoshi and J.J. Novoa, Theoretical analysis of the crystal packing of nitronyl nitroxide radicals: the packing of the α-2-hydro nitronyl nitroxide radical 265 (1997) 190
Deutsch, P.W., L.A. Curtiss and J.P. Blaudeau, Binding energies of germanium clusters, Ge_n ($n = 2$–5) 270 (1997) 413
Devenyi, A., see Mishori, B. 264 (1997) 163
Devriendt, K., H. Van Look, B. Ceursters and J. Peeters, Kinetics of formation of chemiluminescent $CH(A^2\Delta)$ by the elementary reactions of $C_2H(X^2\Sigma^+)$ with $O(^3P)$ and $O_2(X^3\Sigma_g^-)$: a pulse laser photolysis study 261 (1996) 450

De Vries, M.S., see Grannan, S.M. 264 (1997) 359
De Weerd, F., see Moszynski, R. 263 (1996) 107
Dharmasena, K. and M. O'Halloran, On the origin of the CO^+ ion in resonant multiphoton ionization of CO_2 265 (1997) 308
Diamy, A.-M., Z. Randriamanantenasoa, J.-C. Legrand, M. Polisset-Thfoin and J. Fraissard, Use of a dihydrogen plasma afterglow for the reduction of zeolite-supported gold-based metallic catalysts 269 (1997) 327
Dianxun, W., J. Peng and Z. Qiyuan, HeI photoelectron spectrum (PES) of fluorine nitrate, $FONO_2$ 262 (1996) 771
Dianxun, W., Q. Ximei and Z. Shijun, A linear relation between the ionization potentials of HeI photoelectron spectroscopy and NMR chemical shifts. A PES study of the electronic structure of alkyl isocyanides 262 (1996) 776
Díaz-García, M.A., A. Dogariu, D.J. Hagan and E.W. Van Stryland, Nonlinear absorption of soluble octasubstituted metallophthalocyanines at 1.064 μm 266 (1997) 86
Díaz-Herrera, E., see Alvarez-Ramirez, J. 266 (1997) 375
Diestler, D.J., see Schoen, M. 270 (1997) 339
Dietrich, G., see Walther, C. 262 (1996) 668
Dietrich, H., see Schwegmann, S. 264 (1997) 680
Dillet, V., see Adamo, C. 263 (1996) 113
Di Marco, P., see Kalinowski, J. 265 (1997) 607
Dimicoli, I., see Dedonder-Lardeux, C. 264 (1997) 596
DiNardo, N.J., see Plank, R.V. 263 (1996) 33
Ding, C.-F., see Zhu, L. 265 (1997) 177
Ding, G., W. Sun, W. Yang, D. Xu, R. Zhao, G. He and N. Lou, Effects of reagent orbital alignment on product vibrational distributions of the chemiluminescent reaction $Ca(^1P_1) + CH_3I$ 265 (1997) 392
Ding, J., N. Lin, L.-T. Weng, N. Cue and S. Yang, Isolation and characterization of a new metallofullerene $Nd@C_{82}$ 261 (1996) 92
Ding, S. and C.A. McDowell, Shaped pulse excitation in multi-quantum magic-angle spinning spectroscopy of half-integer quadrupole spin systems 270 (1997) 81
Ding, S. and C.A. McDowell, Zeise's salt studied by high resolution solid state ^{13}C CPMAS and ^1H SPEDA NMR spectroscopy 268 (1997) 194
Ding, W., G. Gu, W. Zhong, W.-C. Zang and Y. Du, Enhanced photoluminescence of C_{60} incorporated into interlayers of hydrotalcite 262 (1996) 259
Ding, W., see Gu, G. 270 (1997) 135
Ding, X. and J.C. Wright, Laser-induced fluorescence line-narrowing of C_{60}–hydroquinone crystals 269 (1997) 341
Ding, X., J.M. Alford and J.C. Wright, Lanthanide fluorescence from Er^{3+} in $Er_2@C_{82}$ 269 (1997) 72
Ding, X., see Wu, G. 262 (1996) 421
Dinse, K.-P., see Rübsam, M. 263 (1996) 540
Dirken, P.J., S.C. Kohn, M.E. Smith and E.R.H. van Eck, Complete resolution of Si–O–Si and Si–O–Al fragments in an aluminosilicate glass by ^{17}O multiple quantum magic angle spinning NMR spectroscopy 266 (1997) 568
Dirken, P.J., see Walters, J.K. 264 (1997) 539
Disch, R.L., see Schulman, J.M. 262 (1996) 813
Dlugoborski, T., see Hawlicka, E. 268 (1997) 325
Doan, P.E. and B.M. Hoffman, Making hyperfine selection in Mims ENDOR independent of deadtime 269 (1997) 208

Dobrin, S., see Grabowska, A. 267 (1997) 132
Dobson, K.D., see Duffy, N.W. 266 (1997) 451
Dobson, M.P., see Stace, A.J. 267 (1997) 171
Dods, J., D. Gruner and P. Brumer, A genetic algorithm approach to fitting polyatomic spectra via geometry shifts 261 (1996) 612
Dogariu, A., see Díaz-García, M.A. 266 (1997) 86
Dolg, M., see Shukla, A. 262 (1996) 213
D'Olieslager, J., see Gilliams, B. 269 (1997) 509
Doll, J.D., see Corcelli, S.A. 263 (1996) 671
Domen, K., see Fujino, T. 261 (1996) 534
Donati, A., see Rossi, C. 264 (1997) 205
Dopfer, O., see Meuwly, M. 270 (1997) 252
Dopfer, O., see Nizkorodov, S.A. 265 (1997) 303
Dorn, H.C., see Grannan, S.M. 264 (1997) 359
Doverstål, M., L. Karlsson, B. Lindgren and U. Sassenberg, The $^3\Delta_u$–$X^3\Delta_g$ band system of jet-cooled Ti_2 270 (1997) 273
Dowben, P.A., see McIlroy, D.N. 264 (1997) 168
Doye, J.P.K. and D.J. Wales, The structure of $(C_{60})_N$ clusters 262 (1996) 167
Doye, J.P.K., A. Dullweber and D.J. Wales, Structural predictions for $(C_{60})_N$ clusters with an all-atom potential 269 (1997) 408
Drabbels, M., J.J. ter Meulen and W.L. Meerts, High resolution pulsed-cw double-resonance spectroscopy on the $B\,^1\Sigma^+(v'=0) \leftarrow A\,^1\Pi(v''=0)$ system of CO 267 (1997) 127
Dreassi, E., see Rossi, C. 264 (1997) 205
Dreier, T., see Tadday, R. 268 (1997) 117
Drexhage, K.H., see Müller, R. 262 (1996) 716
Drobizhev, M.A., see Scheblykin, I.G. 261 (1996) 181
Drobizhev, M.A., see Argyrakis, P. 268 (1997) 372
Drouin, B.J., see Sickafoose, S.M. 263 (1996) 191
Droz, T., see Wickleder, C. 264 (1997) 257
Drukker, N., see Saam, B. 263 (1996) 481
Du, X., see Lin, L.-R. 266 (1997) 358
Du, X.-Z., Y.-B. Jiang, L.-R. Lin, X.-Z. Huang and G.-Z. Chen, Phosphorescence-probed study on the association of surfactants with β-cyclodextrin 268 (1997) 31
Du, Y., see Ding, W. 262 (1996) 259
Du, Y., see Gu, G. 270 (1997) 135
Dubois, P., see Agafonov, V. 267 (1997) 193
Duff, J.W. and R.D. Sharma, Quasiclassical trajectory study of the $N(^4S) + NO(X\,^2\Pi) \rightarrow N_2(X\,^1\Sigma_g^+) + O(^3P)$ reaction cross section on the excited $^3A'$ NNO surface 265 (1997) 404
Duffy, N.W., K.D. Dobson, K.C. Gordon, B.H. Robinson and A.J. McQuillan, In situ infrared spectroscopic analysis of the adsorption of ruthenium(II) bipyridyl dicarboxylic acid photosensitisers to TiO_2 in aqueous solutions 266 (1997) 451
Dugourd, P., R.R. Hudgins and M.F. Jarrold, High-resolution ion mobility studies of sodium chloride nanocrystals 267 (1997) 186
Dugourd, Ph., see Antoine, R. 261 (1996) 670
Dujardin, C., see Zhang, L. 268 (1997) 408
Dullweber, A., see Doye, J.P.K. 269 (1997) 408
Duncan, D.I., see Maas, D.J. 270 (1997) 45
Duncan, M.A., see Stangassinger, A. 266 (1997) 189

Duncan, M.A., see Reddic, J.E. 264 (1997) 157
Dunlap, B.I., see Warren, R.W. 262 (1996) 384
Dünser, B., see Senn, G. 266 (1997) 276
Dupuis, B., see Asselin, P. 268 (1997) 265
Durup, J., On the kinetics of infection by pathogenic prion protein molecules 267 (1997) 563
Dutta, C.M., P. Nordlander and M. Kimura, Charge transfer in collisions of an H^+ ion with a ground-state Mg atom at low keV collision energies 264 (1997) 51
Dutton, P.L., see Kumble, R. 261 (1996) 396
Dvinskikh, S.V., G. Buntkowsky, K.M. Salikhov and H.-M. Vieth, Low and zero field stimulated nuclear polarization in cyclic ketones 268 (1997) 401
Dyatko, N.A., M. Capitelli, R. Celiberto and A.P. Napartovich, Attachment rate constants in decaying air plasmas: the role of second kind collisions from electronically excited states 263 (1996) 305
Dyer, M.J., C.G. Bressler and R.A. Copeland, Photodissociation of solid oxygen with tunable ultraviolet laser light: ozone production monitored via Fourier-transform infrared spectroscopy 266 (1997) 548
Dykstra, C.E., see de Oliveira, G. 264 (1997) 85
Dzegilenko, F.N., J.M. Bowman and Y. Amatatsu, Non-Condon effects in photodissociation of ICN($\tilde{A} \leftarrow \tilde{X}$): coupled-channel scattering calculations 264 (1997) 24
Dzuba, S.A., H. Hara, A. Kawamori, M. Iwaki, S. Itoh and Yu.D. Tsvetkov, Electron spin echo of spin-polarised radical pairs in intact and quinone-reconstituted plant photosystem I reaction centres 264 (1997) 238
Dzuba, S.A., P. Gast and A.J. Hoff, Probing the energy landscape of bacterial photosynthetic reaction centers at cryogenic temperatures by ESEEM of spin-polarised $D^+Q_A^-$ radical pairs 268 (1997) 273

Eades, J., see Yamazaki, T. 265 (1997) 137
Earl, W.L., see Labouriau, A. 270 (1997) 278
Eaton, R.A., Y.N.F. Yuan and A. Anderson, Far-infrared spectra of solid methanol at high pressures 269 (1997) 309
Eaton, R.A., see Yuan, Y.N.F. 269 (1997) 305
Echave, J., see Palma, J. 270 (1997) 206
Echt, O., see Matt, S. 264 (1997) 149
Edwards, P.G., see Howard, S.T. 264 (1997) 454
Egawa, C., S. Katayama and S. Oki, Ethylene hydrogenation on a Rh(100) surface 266 (1997) 169
Ehlers, C.J., see Berry, R.J. 269 (1997) 107
Eichelsdörfer, M. and V. Engel, Short-time wave-packet dynamics and the reflection principle of continuum resonance Raman scattering 263 (1996) 640
Eisenmenger, F. and U.H.E. Hansmann, Global minimum configuration of a small peptide for the ECEPP/2 and ECEPP/3 force fields 268 (1997) 86
Elcombe, M., see Gadd, G.E. 261 (1996) 221
Elcombe, M., see Gadd, G.E. 270 (1997) 108
Elkadi, Y. and L. Adamowicz, Dipole-bound anions of ethylene glycol dimers. Theoretical ab initio study 261 (1996) 507
Ellinger, Y., see Talbi, D. 263 (1996) 385
Elokhin, V.I., see Resnyanskii, E.D. 264 (1997) 174
Elsaesser, T., see Chudoba, C. 263 (1996) 622

Elsaesser, T., see Pfeiffer, M. 268 (1997) 258
Enderlein, J., P.M. Goodwin, A. Van Orden, W.P. Ambrose, R. Erdmann and R.A. Keller, A maximum likelihood estimator to distinguish single molecules by their fluorescence decays 270 (1997) 464
Enderlein, J., see Ambrose, W.P. 269 (1997) 365
Endo, S., see Ueda, K. 261 (1996) 295
Eng, R., H.M. Lambert, R. Fei, T. Carrington and S.V. Filseth, Energy disposal in CN(A $^2\Pi$) produced in the 157 nm photodissociation of C_2N_2 261 (1996) 651
Engel, V., see Eichelsdörfer, M. 263 (1996) 640
Engel, V., see Markert, T. 270 (1997) 222
Engeln, R., G. von Helden, G. Berden and G. Meijer, Phase shift cavity ring down absorption spectroscopy 262 (1996) 105
Engeln, R., E. van den Berg, G. Meijer, L. Lin, G.M.H. Knippels and A.F.G. van der Meer, Cavity ring down spectroscopy with a free-electron laser 269 (1997) 293
Engels, B., see Suter, H.U. 261 (1996) 644
Engelsberg, M., see de Souza, I.C.L. 264 (1996) 584
Engkvist, O., G. Karlström and P.O. Widmark, On the origin of the gauche effect. A quantum chemical study of 1,2-difluoroethane 265 (1997) 19
Englman, R., see Baer, M. 265 (1997) 105
Enjo, K., see Maeda, K. 262 (1996) 110
Erdmann, R., see Enderlein, J. 270 (1997) 464
Erickson, R., see Li, H. 266 (1997) 417
Ermolenkov, V.V., see Kruglik, S.G. 270 (1997) 293
Ernst, R.R., see Straus, S.K. 262 (1996) 709
Ernst, R.R., see Brüschweiler, R. 264 (1997) 393
Ernst, R.R., see Mádi, Z.L. 268 (1997) 300
Ernsting, N.P., see Mühlpfordt, A. 263 (1996) 178
Ernzerhof, M., Construction of the adiabatic connection 263 (1996) 499
Ernzerhof, M., see Bündgen, P. 261 (1996) 625
Ernzerhof, M., see Burke, K. 265 (1997) 115
Ertl, G., see Barth, J.V. 270 (1997) 152
Ertl, G., see Mikhailov, A. 267 (1997) 400
Ertl, G., see Schwegmann, S. 264 (1997) 680
Estévez, C.M., see Hass, K.C. 263 (1996) 414
Evans, C.M., J.H. Holloway and A.C. Legon, Rotational spectrum and angular geometry of a pre-reactive complex of oxirane and F_2 267 (1997) 281
Evans, C.M., see Cooke, S.A. 262 (1996) 308
Evans, C.M., see Cotti, G. 264 (1997) 513
Evans, D., see Haran, A. 268 (1997) 475
Evans, P.J., see Gadd, G.E. 261 (1996) 221
Evans, P.J., see Gadd, G.E. 270 (1997) 108
Even, J., M. Bertault, A. Girard, Y. Délugeard and Y. Marqueton, Optical and calorimetric studies on the role of lattice mode softening in assisting a thermally enhanced solid state reaction 267 (1997) 585
Even, U., see Mühlpfordt, A. 263 (1996) 178

Fadley, C.S., see Chambers, S.A. 267 (1997) 51

Faeder, J., N. Delaney, P.E. Maslen and R. Parson, Charge flow and solvent dynamics in the photodissociation of cluster ions: a nonadiabatic molecular dynamics study of $I_2^- \cdot Ar_n$ 270 (1997) 196
Faeder, J., see Maslen, P.E. 263 (1996) 63
Faegri, K., see Saue, T. 263 (1996) 360
Fainberg, B.D., see Zolotov, B. 265 (1997) 418
Fairley, D.A., see Scott, G.B.I. 269 (1997) 88
Fan, K.N., see Huang, H.H. 265 (1997) 508
Fan, S., see Han, W. 265 (1997) 374
Fang, J., J. Wu, X. Lu, Y. Shen and Z. Lu, Sensitization of nanocrystalline TiO_2 electrode with quantum sized CdSe and ZnTCPc molecules 270 (1997) 145
Fang, J.-Y., One step time propagation method for systems with time-dependent Hamiltonians 263 (1996) 759
Färbert, A. and W. Demtröder, Fine and hyperfine structure of the triplet states $1^3\Sigma_u^+$ and $1^3\Sigma_g^+$ of the Na_2 molecule 264 (1997) 225
Faria, R.M., see Mergulhão, S. 269 (1997) 489
Fattori, V., see Kalinowski, J. 265 (1997) 607
Faulkner, S., see Beeby, A. 266 (1997) 116
Favero, L.B., see Caminati, W. 265 (1997) 561
Favero, P.G., see Caminati, W. 265 (1997) 561
Favero, P.G., see Melandri, S. 261 (1996) 267
Favero, P.G., see Caminati, W. 268 (1997) 393
Fedorov, A., M.N. Berberan-Santos, J.-P. Lefèvre and B. Valeur, Picosecond time-resolved and steady-state studies of the polarization of the fluorescence of C_{60} and C_{70} 267 (1997) 467
Fehér, M. and P.A. Martin, Ab initio calculation of the electrical properties of the $X^2\Pi_g$ ground state of O_2^+ 261 (1996) 23
Fei, R., see Eng, R. 261 (1996) 651
Feldstein, M.J., see Wang, W. 262 (1996) 573
Fender, B. and P.R. Callis, ^1L_a origin locations of methyl indoles in argon matrices 262 (1996) 343
Feng, J., see Ge, M. 264 (1997) 139
Feng, P.Y. and K. Balasubramanian, Electronic states and potential energy curves of Ga_2P, GaP_2, and their ions 265 (1997) 41
Feng, P.Y. and K. Balasubramanian, Nearly-degenerate electronic states for Ga_3P_2 and Ga_2P_3 265 (1997) 547
Feng, P.Y. and K. Balasubramanian, Geometries and energy separations of the electronic states of In_2P_2 264 (1997) 449
Feng, W.L., Y. Wang, S.W. Zhang and X.Y. Pang, Theoretical investigation of the mechanism and kinetics for HCO + HCN ⇄ HCHO + CN 266 (1997) 43
Ferguson, E.E., see Le Garrec, J.L. 270 (1997) 66
Feries, J., see Deren, P.J. 264 (1997) 614
Fernández, A., see Soriano, L. 266 (1997) 184
Fernández, J.A., I. Merelas, D. Husain, M.N. Sánchez Rayo and F. Castaño, Direct measurements of removal rates of electronically excited $NCO(\tilde{A}^2\Sigma^+(0,0,0))$ by simple molecules 267 (1997) 301
Fernández Cézar, R., see del Barrio, J.I. 270 (1997) 71
Ferraro, G., see Laganà, A. 267 (1997) 403
Ferris, K., see Chambers, S.A. 267 (1997) 51
Figueirido, F.E., see Del Buono, G.S. 263 (1996) 521

Filseth, S.V., see Eng, R. 261 (1996) 651
Finger, K. and P. Saalfrank, Vibrationally excited products after the photodesorption of NO from Pt(111): a two-mode open-system density matrix approach 268 (1997) 291
Fink, R., see Gebauer, W. 266 (1997) 177
Fischer, G., X. Cao and R.L. Purchase, FT-IR spectrum of the 2H-tautomer of benzotriazole in a supersonic jet 262 (1996) 689
Fischer, S.F., see Zharikov, A.A. 263 (1996) 749
Fischer, S.F., see Scherer, P.O.J. 268 (1997) 133
Fisher, E.R., see Bogart, K.H.A. 267 (1997) 377
Fisher, T.A., see Lidzey, D.G. 263 (1996) 655
Fisz, J.J. and A. van Hoek, Picosecond emission anisotropy decays of dimethyl aminobenzonitrile 270 (1997) 432
Fisz, J.J., Polarized fluorescence decay surface for many-ground- and many-excited-state species in solution 262 (1996) 507
Fisz, J.J., Polarized fluorescence spectroscopy of two-ground- and two-excited-state systems in solutions 262 (1996) 495
Fisz, J.J., Time-resolved polarized fluorescence spectroscopy of photoreactive systems in uniaxially organized molecular media 269 (1997) 244
Flament, J.P., see Robbe, J.M. 267 (1997) 91
Flammang, R., see Lahem, D. 270 (1997) 93
Fleming, J., see Medhurst, L.J. 266 (1997) 607
Fleming, P.E., see Lorenz, K.T. 261 (1996) 145
Fletcher, T.R., see Ravichandran, K. 261 (1996) 261
Fleury, L., see Wrachtrup, J. 267 (1997) 179
Flores, J.R., On the accuracy of second-order Møller–Plesset correlation energies 270 (1997) 427
Fogarasi, G., see Szalay, P.G. 263 (1996) 91
Fogarasi, G., see Szalay, P.G. 270 (1997) 406
Fonseca, T.L., see de Melo, C.P. 261 (1996) 28
Foreman, J.P., see Howard, S.T. 264 (1997) 454
Forst, W., Approximations for angular momentum-conserved polyatomic vibrational–rotational sum and density of states under a central potential 262 (1996) 539
Fowler, P.W., see Seifert, G. 268 (1997) 352
Fox, R.W., see Rudich, Y. 261 (1996) 467
Fraissard, J., see Diamy, A.-M. 269 (1997) 327
Francisco, J.S., Ab initio study on the potential energy hypersurface of $FC(O)O^+$ 265 (1997) 521
Francisco, J.S., see Good, D.A. 266 (1997) 512
Francisco, J.S., see L.Richardson, S. 270 (1997) 395
Franke, R., Numerical study of the iterative solution of the one-electron Dirac equation based on 'direct perturbation theory' 264 (1997) 495
Frankevich, E.L., G.E. Zoriniants, A.N. Chaban, M.M. Triebel, S. Blumstengel and V.M. Kobryanskii, Magnetic field effects on photoluminescence in PPP. Investigation of the influence of chain length and degree of order 261 (1996) 545
Frantsuzov, P.A., The failure of the diffusional description of the level crossing problem. I. Violation of the von Neumann conditions 267 (1997) 427
Frantsuzov, P.A., see Burshtein, A.I. 263 (1996) 513
Frauenheim, Th., see Seifert, G. 268 (1997) 352
Freed, J.H., see Salikhov, K.M. 262 (1996) 17
Freed, J.H., see Salikhov, K.M. 265 (1997) 562

Freeman, C.G., see Scott, G.B.I. 269 (1997) 88
Frei, H., see Kauffmann, E. 266 (1997) 554
Freudenberg, Th., V. Stert, W. Radloff, J. Ringling, J. Güdde, G. Korn and I.V. Hertel, Ultrafast dynamics of ammonia clusters excited by femtosecond VUV laser pulses 269 (1997) 523
Freudenberg, Th., see Radloff, W. 261 (1996) 301
Freudenberg, Th., see Radloff, W. 264 (1997) 210
Frey, H.-M., see Radi, P.P. 265 (1997) 271
Friedrich, B. and D. Herschbach, Alignment enhanced spectra of molecules in intense non-resonant laser fields 262 (1996) 41
Friesen, L.A., see Larson, E.J. 265 (1997) 161
Frioud, M., see Daul, C. 262 (1996) 74
Frischkorn, C., see Baumfalk, R. 269 (1997) 321
Frishman, A., see Hoffman, D.K. 262 (1996) 393
Fritzsche, S., R. Haberlandt, G. Hofmann, J. Kärger, K. Heinzinger and M. Wolfsberg, An MD study on the diffusion of methane in a cation-free LTA zeolite. Illustrations and new results 265 (1997) 253
Froese, R.D.J. and K. Morokuma, The IMOMO and IMOMM methods for excited states. A study of the adiabatic $S_0 \rightarrow T_{1,2}$ excitation energies of cyclic alkenes and enones 263 (1996) 393
Frost, M.J., see Payne, M.A. 265 (1997) 244
Fu, R., P. Pelupessy and G. Bodenhausen, Frequency-modulated cross-polarization for fast magic angle spinning NMR at high fields: relaxing the Hartmann–Hahn condition 264 (1997) 63
Fuchs, D., see Cummins, T.R. 261 (1996) 228
Fuchs, O.L., see Braun, E. 265 (1997) 434
Fuhrmann, D., see Witte, G. 265 (1997) 347
Fujii, A., see Maeyama, T. 264 (1997) 292
Fujii, T. and H.S. Kim, Mass spectrometric analysis of the neutral products in a C_2H_4 microwave plasma: carbon carbenes and aromatic compounds 268 (1997) 229
Fujimori, K., see Uchimaru, T. 267 (1997) 244
Fujimura, Y., see Alexander, A.J. 262 (1996) 589
Fujimura, Y., see Fujiwara, T. 261 (1996) 201
Fujino, T., M. Kashitani, K. Fukuyama, J. Kubota, J.N. Kondo, A. Wada, K. Domen, C. Hirose, F. Wakabayashi and S.S. Kano, Population lifetimes of the OH stretching band of water molecules on zeolite surfaces 261 (1996) 534
Fujita, T., see Hidaka, M. 264 (1997) 371
Fujita, Y., see Yamazaki, T. 265 (1997) 137
Fujiwara, T., Y. Fujimura and O. Kajimoto, Rotational coherence spectroscopy of 9,9′-bianthryl and its van der Waals complexes with Ar and H_2O 261 (1996) 201
Fujiwara, Y., see Harima, Y. 267 (1997) 481
Fuke, K., see Hashimoto, K. 266 (1997) 7
Fukumi, T., see Kamada, K. 263 (1996) 215
Fukumi, T., see Kamada, K. 267 (1997) 402
Fukuyama, K., see Fujino, T. 261 (1996) 534
Fulde, P., see Shukla, A. 262 (1996) 213
Füller, T., see Banhart, F. 269 (1997) 349
Furlani, A., see Polzonetti, G. 267 (1997) 384
Furlani, C., see Polzonetti, G. 267 (1997) 384
Furukawa, Y., see Hirata, S. 261 (1996) 241

Fuß, W., T. Schikarski, W.E. Schmid, S. Trushin and K.L. Kompa, Ultrafast dynamics of the photochemical ring opening of 1,3-cyclohexadiene studied by multiphoton ionization 262 (1996) 675
Fusina, L., see Bürger, H. 268 (1997) 249
Fuss, W., see Kwok, W.M. 261 (1996) 685

G-Tablas, F.M., see del Barrio, J.I. 270 (1997) 71
Gabuda, S.P., S.G. Kozlova and R.L. Davidovich, Novel-type chemical bonding in TlF due to $6s^2$ inert pair activation 263 (1996) 253
Gadd, G.E., P.J. Evans, D.J. Hurwood, J. Wood, S. Moricca, M. Blackford, M. Elcombe, S. Kennedy and M. James, Neutron irradiation of Ar_1C_{60} 261 (1996) 221
Gadd, G.E., P.J. Evans, D.J. Hurwood, P.L. Morgan, S. Moricca, N. Webb, J. Holmes, G. McOrist, T. Wall, M. Blackford, D. Cassidy, M. Elcombe, J.T. Noorman, P. Johnson and P. Prasad, Endohedral fullerene formation through prompt gamma recoil 270 (1997) 108
Galaup, J.P., see Arabei, S.M. 270 (1997) 31
Galievsky, V.A., see Kruglik, S.G. 270 (1997) 293
Gallagher, H.G., see Qi, X. 264 (1997) 623
Gallo, D., see Bosi, L. 267 (1997) 123
Gal'pern, E.G., I.V. Stankevich, A.L. Chistyakov and L.A. Chernozatonskii, Models of the stable dumbbell-like C_{120} cluster and crimped nanotubes constructed from C_{60} fullerenes 269 (1997) 85
Galvão, D.S., see Baughman, R.H. 269 (1997) 356
Gammie, D.I., see Carrington, A. 262 (1996) 598
Gan, A., see Zolotov, B. 265 (1997) 418
Gandhi, S.R., see Baumfalk, R. 269 (1997) 321
Gao, J.S. and Z.Q. Tian, Surface enhanced Raman scattering of pyridine at copper electrodes excited with a 514.5 nm line 262 (1996) 151
Gao, R., see Shang, H. 267 (1997) 345
Garashchuk, S. and D. Tannor, Wave packet correlation function approach to $H_2(v) + H \rightarrow H + H_2(v')$: semiclassical implementation 262 (1996) 477
Garashchuk, S. and D.J. Tannor, Calculation of autocorrelation functions using the Wigner representation of quantum mechanics 263 (1996) 324
Garay, M., see de Castro Vítores, M. 263 (1996) 456
García, G., M. Roteta and F. Manero, Electron scattering by N_2 and CO at intermediate energies: 1–10 keV 264 (1997) 589
García, V.M., R. Caballol and J.P. Malrieu, Theoretical study of the ethylene electronic spectrum and extraction of an *r*-dependent Hubbard Hamiltonian 261 (1996) 98
Garrett, W.R., see Deng, L. 270 (1997) 299
Gast, P., see Spoyalov, A.P. 263 (1996) 715
Gast, P., see Dzuba, S.A. 268 (1997) 273
Gatt, R., see Panas, I. 266 (1997) 410
Gatt, R., see Panas, I. 270 (1997) 178
Gauld, J.W., M.N. Glukhovtsev and L. Radom, The structure of the methanol radical cation: an artificially short C–O bond with MP2 theory 262 (1996) 187
Gauss, J., see Christiansen, O. 266 (1997) 53
Gauss, J., see Stanton, J.F. 262 (1996) 183
Ge, M., J. Feng, X. Huang, C. Yang and C. Sun, Ab initio study on Mo_2C_8 cluster 264 (1997) 139
Gebauer, W., M. Bässler, R. Fink, M. Sokolowski and E. Umbach, New insight into the optical properties of thin organic films by epitaxial preparation 266 (1997) 177
Geerlings, P., see De Proft, F. 262 (1996) 782

Geerlings, P., see Verbandt, Y. 270 (1997) 471
Geissler, M., see Grummt, U.-W. 263 (1996) 581
Gejo, T., H. Bitto and J.R. Huber, Quantum beats in the S_1 dynamics of acetaldehyde 261 (1996) 443
Gelinck, G.H., J.M. Warman, M. Remmers and D. Neher, Narrow-band emissions from conjugated-polymer films 265 (1997) 320
Gellini, C., P.R. Salvi, V. Schettino and H.J. Jodl, Three-phonon vibrational complexes in crystal N_2O 268 (1997) 381
Geng, J., T. Kobayashi and M. Takami, High Rydberg states of the NO molecule studied by two-color four-wave mixing spectroscopy 266 (1997) 290
Georgiou, S., A. Koubenakis, M. Syrrou and P. Kontoleta, The importance of the plume ejection time for the fragmentation yields observed in the UV ablation of molecular van der Waals films. Ablation of chlorobenzene films at 248 nm 270 (1997) 491
Gerber, G., see Bañares, L. 267 (1997) 141
Gerber, T., see Radi, P.P. 265 (1997) 271
Gerhard-Multhaupt, R., see Bauer-Gogonea, S. 262 (1996) 663
Gerhards, M., see Schumm, S. 263 (1996) 126
Gervasi, O., see Laganà, A. 267 (1997) 403
Gfeller, S., see Bitto, H. 265 (1997) 600
Ghedini, M., D. Pucci, G. Calogero and F. Barigelletti, Luminescence of azobenzene derivatives induced by cyclopalladation 267 (1997) 341
Gherghel, L., see Baumgarten, M. 267 (1997) 175
Ghiggino, K.P., see Bell, T.D.M. 268 (1997) 223
Ghosh, A.S., see Adhikari, S.K. 262 (1996) 460
Ghosh, H.N., D.K. Palit, A.V. Sapre and J.P. Mittal, Charge separation, charge recombination and electron transfer reactions in solutions of fullerene-C_{60} and phenothiazines 265 (1997) 365
Ghosh, S., see Bhattacharyya, S. 269 (1997) 314
Giannozzi, P., see Lorentzen, J.D. 270 (1997) 129
Giebel, U., see Smith, B.A. 270 (1997) 139
Gier, H., see Schumm, S. 263 (1996) 126
Giering, T. and D. Haarer, Structural relaxations in amorphous water studied by hole-burning spectroscopy 261 (1996) 677
Giesa, S., see Gromov, A. 267 (1997) 460
Gil-Villegas, A., S.C. McGrother and G. Jackson, Chain and ring structures in smectic phases of molecules with transverse dipoles 269 (1997) 441
Gilbert, S.E., see Cavalleri, O. 269 (1997) 479
Gill, P.M.W. and R.D. Adamson, A family of attenuated Coulomb operators 261 (1996) 105
Gill, P.M.W., A new expansion of the Coulomb interaction 270 (1997) 193
Gillan, M.J., see Andrews, S.B. 261 (1996) 521
Gillan, M.J., see Lindan, P.J.D. 261 (1996) 246
Gilliams, B., J.-Y. Tilquin, L. Heerman, J. D'Olieslager and C. Görller-Walrand, Evidence for Rh(II) in a LiCl–KCl eutectic. An optical absorption investigation 269 (1997) 509
Gimzewski, J.K., see Joachim, C. 265 (1997) 353
Giordano, D., see Capitelli, M. 263 (1996) 635
Girard, A., see Even, J. 267 (1997) 585
Girardet, C., see Iglesias-Groth, S. 264 (1997) 351
Giro, G., see Kalinowski, J. 265 (1997) 607
Gladenkova, S.N., see Osad'ko, I.S. 270 (1997) 183
Glasbeek, M., see Middelhoek, E.R. 267 (1997) 525

Glukhovtsev, M.N. and R.D. Bach, Ab initio study on the thermochemistry of diphosphine (P_2H_4) and diphosphine radical cation ($P_2H_4^{+\cdot}$) 265 (1997) 514
Glukhovtsev, M.N. and R.D. Bach, Methylene–iodonium ylide: an isomer of diiodomethane 269 (1997) 145
Glukhovtsev, M.N., see Gauld, J.W. 262 (1996) 187
Glushkov, V.N. and A.Ya. Tsaune, Ab initio calculation of excited state energies using basis set optimization and open-shell Møller–Plesset perturbation theory 262 (1996) 59
Gobbato, K.I., S.E. Ulic, C.O. Della Védova, H.-G. Mack and H. Oberhammer, (Fluorocarbonyl)sulfenyl isocyanate, FC(O)SNCO: unusual conformational properties 266 (1997) 527
Godoy, S., see Braun, E. 265 (1997) 434
Goebel, D. and U. Hohm, Dispersion of the mean dipole polarizability $\alpha(\omega)$ and dipole polarizability anisotropy $\kappa(\omega)$ of bromotrifluoromethane $CBrF_3$ 265 (1997) 638
Goh, S.K. and A. St-Amant, Using a fitted electronic density to improve the efficiency of a linear combination of Gaussian-type orbitals calculation 264 (1997) 9
Gołąb, S., see Ryba-Romanowski, W. 264 (1997) 323
Golde, M.F., see Gougousi, T. 265 (1997) 399
Golding, B., see Kim, J.U. 267 (1997) 323
Goldschleger, A.U., E.Ya. Misochko, A.V. Akimov, I.U. Goldschleger and V.A. Benderskii, Formation of the H–HF complex in the reaction of thermal fluorine atoms with hydrogen molecules in solid Ar 267 (1997) 288
Goldschleger, I.U., see Goldschleger, A.U. 267 (1997) 288
Gomei, M., see Negishi, Y. 269 (1997) 199
Gómez, U., M. Leonhardt, H. Port and H.C. Wolf, Optical properties of amorphous ultrathin films of perylene derivatives 268 (1997) 1
Gomez Llorente, J.M., see Ruiz, A. 270 (1997) 121
Gondal, M.A., see Khan, M.A. 264 (1997) 273
González-Elipe, A.R., see Soriano, L. 266 (1997) 184
González, L., O. Mó and M. Yáñez, High-level ab initio calculations on the 1,2-dithioglyoxal/1,2-dithiete isomerism 263 (1996) 407
Gonzalez-Lezana, T., see Buchachenko, A.A. 269 (1997) 448
Good, D.A. and J.S. Francisco, Heat of formation of CH_3OCH_2 radical 266 (1997) 512
Goodman, D.W., see Xu, C. 263 (1996) 13
Goodman, D.W., see Xu, C. 265 (1997) 341
Goodson, D.Z., see Suvernev, A.A. 269 (1997) 177
Goodwin, P.M., see Enderlein, J. 270 (1997) 464
Goodwin, P.M., see Ambrose, W.P. 269 (1997) 365
Gopidas, K.R., see Manoj, N. 267 (1997) 567
Gordon, K.C., see Duffy, N.W. 266 (1997) 451
Gorelik, V.R., see Bagryanskaya, E.G. 264 (1997) 655
Görller-Walrand, C., see Binnemans, K. 266 (1997) 297
Görller-Walrand, C., see Gilliams, B. 269 (1997) 509
Gorse, C., see Capitelli, M. 263 (1996) 635
Gorte, R.J., see Šepa, J. 262 (1996) 321
Gottlieb, C.A., see McCarthy, M.C. 264 (1997) 252
Gougousi, T., M.F. Golde and R. Johnsen, Electron–ion recombination rate coefficient measurements in a flowing afterglow plasma 265 (1997) 399
Gould, I.R., see Scholes, G.D. 266 (1997) 521
Govindaraj, A., see Sen, R. 267 (1997) 276

Grabowska, A., K. Kownacki, J. Karpiuk, S. Dobrin and Ł. Kaczmarek, Photochromism and proton transfer reaction cycle of new internally H-bonded Schiff bases 267 (1997) 132
Graf, S., see Sabo, D. 261 (1996) 318
Graf, U., see Niikura, H. 266 (1997) 217
Grahn, W., see Werncke, W. 266 (1997) 99
Grandinetti, F., see Aschi, M. 267 (1997) 98
Grannan, S.M., J.T. Birmingham, P.L. Richards, D.S. Bethune, M.S. de Vries, P.H.M. van Loosdrecht, H.C. Dorn, P. Burbank, J. Bailey and S. Stevenson, Far infrared transmittance of $Sc_2@C_{84}$ and $Er_2@C_{82}$ 264 (1997) 359
Gregory, J.K., see Sorenson, J.M. 263 (1996) 680
Grein, F., see Bündgen, P. 261 (1996) 625
Griffiths, I.W., see Jeffreys, N. 266 (1997) 537
Griffiths, P.T., see Simpson, C.J.S.M. 263 (1996) 19
Grigorenko, B.L. and A.V. Nemukhin, Modelling trapping sites of $(HF)_2$ in argon clusters 270 (1997) 103
Grigoryan, L.S., see Nakashima, S. 268 (1997) 359
Grill, V., see Wörgötter, R. 270 (1997) 333
Grill, V., see Matt, S. 264 (1997) 149
Grimley, T.B., see Brivio, G.P. 263 (1996) 597
Grinevich, O. and D.L. Snavely, Vibrational overtone enhancement of methyl methacrylate polymerization initiated by benzoyl peroxide decomposition 267 (1997) 313
Groenen, E.J.J., see Warntjes, J.B.M. 261 (1996) 495
Groenenboom, G.C., see Moszynski, R. 263 (1996) 107
Gromov, A., S. Ballenweg, S. Giesa, S. Lebedkin, W.E. Hull and W. Krätschmer, Preparation and characterisation of C_{119} 267 (1997) 460
Grönbeck, H. and W. Andreoni, Theoretical study of $(CO)_n$ chemisorption on Pt and Pt_3: structural, electronic and vibrational properties 269 (1997) 385
Grönbeck, H., D. Tománek, S.G. Kim and A. Rosén, Does hydrogen pre-melt palladium clusters? 264 (1997) 39
Groot, T., see Berden, G. 265 (1997) 204
Gropen, O., see Saue, T. 263 (1996) 360
Gross, A. and M. Scheffler, Scattering of hydrogen molecules from a reactive surface: strong off-specular and rotationally inelastic diffraction 263 (1996) 567
Grossmann, F., Time-dependent semiclassical calculation of resonance lifetimes 262 (1996) 470
Grosswasser, D., see Rosenblum, G. 263 (1996) 441
Gruber, A., see Wrachtrup, J. 267 (1997) 179
Gruber, D., see Li, X. 263 (1996) 463
Gruenloh, C., see Pribble, R.N. 262 (1996) 627
Grummt, U.-W., M. Geissler and Th. Schmitz-Huebsch, Chemical deposition of silver nanoclusters on self-assembled organic monolayers. A strategy to contact individual molecules 263 (1996) 581
Gruner, D., see Dods, J. 261 (1996) 612
Gu, B., see Han, W. 265 (1997) 374
Gu, G., W. Ding, G. Cheng, S. Zhang, Y. Du and S. Yang, Photoluminescence studies on C_{60} trapped in NiY zeolite 270 (1997) 135
Gu, G., see Ding, W. 262 (1996) 259
Güdde, J., see Freudenberg, Th. 269 (1997) 523
Güdel, H.U., see Hazenkamp, M.F. 265 (1997) 264
Güdel, H.U., see Weihe, H. 261 (1996) 123

Güdel, H.U., see Brunold, T.C. 268 (1997) 413
Gudipati, M.S. and M. Kalb, Energy transfer involving higher excited states: a comparison between CO ... anthracene and O_2 ... anthracene in Ar matrices 268 (1997) 169
Guenneau, F., see Canet, D. 264 (1996) 477
Guérin, H., Supersymmetric WKB and WKB s wave phase shifts for the Morse potential 262 (1996) 759
Guha, S., see Lorentzen, J.D. 270 (1997) 129
Guillot, B., see Cabaco, M.I. 262 (1996) 120
Guissani, Y., see Cabaco, M.I. 262 (1996) 120
Guldi, D.M., see Staško, A. 262 (1996) 233
Guo, B., see Colarusso, P. 269 (1997) 39
Guo, H., see Chen, R. 261 (1996) 605
Guo, L.P., Y. Chen, E.G. Wang, L. Li and Z.X. Zhao, Identification of a new C–N phase with monoclinic structure 268 (1997) 26
Guo, Z., see Li, Y. 265 (1997) 361
Gupta, Y.M., see Russell, T.P. 267 (1997) 351
Gutsev, G.L. and R.J. Bartlett, Electron affinity of NH: a coupled-cluster and Hartree–Fock density-functional-theory study 265 (1997) 12
Gwóźdź, E., A. Bródka and K. Pasterny, Molecular dynamics simulation study of a liquid crystal model: Gay–Berne particles with transverse dipole moments 267 (1997) 557

Haaland, P., see Jiao, C.Q. 265 (1997) 239
Haaland, P.D., see Jiao, C.Q. 269 (1997) 117
Haarer, D., see Giering, T. 261 (1996) 677
Haase, F., J. Sauer and J. Hutter, Ab initio molecular dynamics simulation of methanol adsorbed in chabazite 266 (1997) 397
Haberlandt, R., see Fritzsche, S. 265 (1997) 253
Hachimi, A. and J.F. Muller, Chromium cluster formation under resonant and non-resonant laser ablation 268 (1997) 485
Hada, M., H. Kaneko and H. Nakatsuji, Relativistic study of nuclear magnetic shielding constants: tungsten hexahalides and tetraoxide 261 (1996) 7
Hada, M., see Kaneko, H. 261 (1996) 1
Hadj Bachir, I., T.R. Huet, J.L. Destombes and M. Vervloet, Laser optogalvanic spectroscopy of N_2 from the $A^3\Sigma_u^+$ metastable state in a corona excited supersonic expansion 270 (1997) 533
Haensler, M., see Volke, F. 262 (1996) 374
Hagan, D.J., see Díaz-García, M.A. 266 (1997) 86
Hagiwara, K., see Imahori, H. 263 (1996) 545
Hahn, J.W., see Kim, D.-C. 265 (1997) 573
Hain, T.D., M.A. Weibel, K.M. Backstrand, P.E. Pope and T.J. Curtiss, State-selected beams of hydroxyl radicals via electric hexapole focusing 262 (1996) 723
Hall, G.E., see North, S.W. 263 (1996) 148
Hamaguchi, H., see Ishibashi, T. 264 (1997) 551
Hamaguchi, H.-o., see Iwata, K. 261 (1996) 208
Hamai, S., Dual fluorescence of 2-naphthalenecarboxylic acid in water–organic solvent mixtures 267 (1997) 515
Hamanaka, Y., see Kotani, S. 269 (1997) 274
Hamanaka, Y., see Nakashima, S. 268 (1997) 359

Hamanoue, K., T. Nakayama, Y. Amijima and K. Ibuki, A rapid decay channel of the lowest excited singlet state of 9-benzoyl-10-nitroanthracene generating 9-benzoyl-10-anthryloxy radical and nitrogen (II) oxide 267 (1997) 165
Hamanoue, K., see Nakayama, T. 266 (1997) 601
Hamilton, P.A., A.J. Phillips and R. Windsor, Determination of the hyperfine structure of the $B\,^2\Pi_{1/2}$ state of NO from quantum beat spectroscopy 264 (1997) 245
Hamm, P., M. Zurek, T. Röschinger, H. Patzelt, D. Oesterhelt and W. Zinth, Femtosecond spectroscopy of the photoisomerisation of the protonated Schiff base of all-trans retinal 263 (1996) 613
Hamm, P., M. Zurek, T. Röschinger, H. Patzelt, D. Oesterhelt and W. Zinth, Subpicosecond infrared spectroscopy on the photoisomerisation of the protonated Schiff base of all-trans retinal 268 (1997) 180
Hammes-Schiffer, S., see Morelli, J. 269 (1997) 161
Han, J., A.L. McIntosh, Z. Wang, R.R. Lucchese and J.W. Bevan, Intermolecular potential for Ar–HBr ($\nu_1 = 1$) studied by high resolution near infrared spectroscopy 265 (1997) 209
Han, J., A.L. McIntosh, C.L. Hartz and J.W. Bevan, A rovibrational analysis of the ν_1 and ν_2 bands of OC–DF by supersonic jet FTIR spectroscopy 264 (1997) 411
Han, K.-L., see Zhan, J.-P. 264 (1997) 687
Han, P., see Werst, D.W. 269 (1997) 333
Han, T.P.J., see Qi, X. 264 (1997) 623
Han, W., S. Fan, Q. Li, W. Liang, B. Gu and D. Yu, Continuous synthesis and characterization of silicon carbide nanorods 265 (1997) 374
Han, Y.-K., see Jeong, H.Y. 263 (1996) 345
Hancock, G., see Ball, S.M. 264 (1997) 531
Handy, N.C., see Neumann, R. 266 (1997) 16
Handy, N.C., see Tozer, D.J. 265 (1997) 614
Hannongbua, S., see Aree, T. 266 (1997) 427
Hansmann, U.H.E., see Eisenmenger, F. 268 (1997) 86
Happer, W., see Saam, B. 263 (1996) 481
Hara, H., see Dzuba, S.A. 264 (1997) 238
Hara, R., see Uchimaru, T. 267 (1997) 244
Harada, K., see Ishiguro, M. 263 (1996) 629
Haran, A., A. Kadyshevitch, H. Cohen, R. Naaman, D. Evans, T. Seideman and A. Nitzan, Electron transmission through band structure in organized organic thin films 268 (1997) 475
Haran, G., K. Wynne, A. Xie, Q. He, M. Chance and R.M. Hochstrasser, Excited state dynamics of bacteriorhodopsin revealed by transient stimulated emission spectra 261 (1996) 389
Hare, J.P., see Hsu, W.K. 262 (1996) 161
Harima, H., see Nakashima, S. 268 (1997) 359
Harima, Y., M. Miyatake, P. Price and K. Yamashita, Photoresponse of porphyrin thin-film electrode in the near-infrared 262 (1996) 274
Harima, Y., T. Kodaka, Y. Kunugi, K. Yamashita, Y. Akimoto, Y. Fujiwara and Y. Tanimoto, Phosphorescence and S–T absorption in vanadyl(IV) tetraphenylporphyrin at room temperature 267 (1997) 481
Harris, F.M., see Jeffreys, N. 266 (1997) 537
Harris, F.M., see Silcocks, S.E. 262 (1996) 355
Harris, R.A., see Maierle, C.S. 267 (1997) 199
Harris, R.K., see Scheler, U. 262 (1996) 137
Harrison, J.F., see Rencsok, R. 262 (1996) 207
Harrison, N.M., B.G. Searle and E.A. Seddon, An ab initio study of the magnetic coupling in bi-metallic Cr^{III} cyanides 266 (1997) 507

Harrison, N.M., see Lindan, P.J.D. 261 (1996) 246
Hartmann, F.J., see Yamazaki, T. 265 (1997) 137
Hartmann, J.M., see Ozanne, L. 261 (1996) 353
Hartmann, W.K., see Kim, J.U. 267 (1997) 323
Hartz, C.L., see Han, J. 264 (1997) 411
Häser, M., see Bauernschmitt, R. 264 (1996) 573
Hashimoto, F., see Waga, M. 265 (1997) 277
Hashimoto, K., T. Kamimoto and K. Fuke, Ab initio MO study of solvated negative alkali atom clusters: $[M(H_2O)_n]^-$ and $[M(NH_3)_n]^-$ (M = Na and Li, $n = 1–3$) 266 (1997) 7
Hashimoto, N., N. Yonekura and T. Suzuki, Pump–probe measurements of the predissociation reaction time of C_2H_2 from $\tilde{A}(^1A_u)$ state 264 (1997) 545
Hashimoto, S., Observation of charge-resonance band of naphthalene dimer cation confined in cavities of faujasite zeolites. Near-IR diffuse reflectance laser photolysis study 262 (1996) 292
Hasinoff, M., see Yamazaki, T. 265 (1997) 137
Hass, K.C., W.F. Schneider, C.M. Estévez and R.D. Bach, Density functional theory description of excited-state intramolecular proton transfer 263 (1996) 414
Hatrick, D.A., see Volkmer, A. 268 (1997) 439
Hättig, C., O. Christiansen, H. Koch and P. Jørgensen, Frequency-dependent first hyperpolarizabilities using coupled cluster quadratic response theory 269 (1997) 428
Hättig, C., On the calculation of derivatives for Coulomb-type interaction energies and general anisotropic pair potentials 268 (1997) 521
Hauser, A., H. Riesen, R. Pellaux and S. Decurtins, Resonant excitation energy transfer in $[Rh(bpy)_3][NaCr(ox)_3]ClO_4$ 261 (1996) 313
Hawlicka, E. and T. Dlugoborski, Molecular dynamics simulations of the aqueous solution of tetramethylammonium chloride 268 (1997) 325
Hayakawa, F., see Negishi, Y. 269 (1997) 199
Hayano, R.S., see Yamazaki, T. 265 (1997) 137
Hayase, T., see Negishi, Y. 269 (1997) 199
Hayashi, H., see Nishizawa, K. 267 (1997) 501
Hayden, B.E., A. King and M.A. Newton, The alignment of a surface species determined by FT-RAIRS: rhodium gem–dicarbonyl on $TiO_2(110)$ 269 (1997) 485
Hayes, T., D. Bellert, T. Buthelezi and P.J. Brucat, The photodissociation of $V^+ \cdot CH_4$ 264 (1997) 220
Hayes, T., see Buthelezi, T. 262 (1996) 303
Hazenkamp, M.F., H.U. Güdel, S. Kück, G. Huber, W. Rauw and D. Reinen, Excited state absorption and laser potential of Mn^{5+}-doped Li_3PO_4 265 (1997) 264
He, G., see Ding, G. 265 (1997) 392
He, G.-Z., see Zhan, J.-P. 264 (1997) 687
He, Q., see Haran, G. 261 (1996) 389
He, T., see Li, L. 262 (1996) 52
He, T., see Li, L. 268 (1997) 549
Head-Gordon, M., see Ochsenfeld, C. 270 (1997) 399
Healy, D., see Cross, G.H. 268 (1997) 36
Hedgecock, I.M., see Naulin, C. 266 (1997) 335
Hedhili, M.N., R. Azria, Y. Le Coat and M. Tronc, O^- ESD dynamics from condensed N_2O 268 (1997) 21
Heeger, A.J., see Schwartz, B.J. 265 (1997) 327
Heerman, L., see Gilliams, B. 269 (1997) 509
Heine, V., see Lee, M.-H. 265 (1997) 673

Heinzinger, K., see Fritzsche, S. 265 (1997) 253
Held, A., L.Ya. Baranov, H.L. Selzle and E.W. Schlag, The interactions of a ZEKE electron with its ionic core: an experimental measurement 267 (1997) 318
Helgaker, T., see Christiansen, O. 263 (1996) 530
Helgaker, T., see Ruud, K. 264 (1997) 17
Hellingwerf, K.J., see Baltuška, A. 270 (1997) 263
Helm, R.M., H.-P. Vogel and H.J. Neusser, Highly resolved UV spectroscopy: structure of S_1 benzonitrile and benzonitrile–argon by correlation automated rotational fitting 270 (1997) 285
Hemmingsen, T., see Treindl, L. 269 (1997) 263
Henari, F.Z., W.J. Blau, L.R. Milgrom, G. Yahioglu, D. Phillips and J.A. Lacey, Third-order optical non-linearity in Zn(II) complexes of 5,10,15,20-tetraarylethynyl-substituted porphyrins 267 (1997) 229
Henderson, B., see Qi, X. 264 (1997) 623
Henderson, D., see Trokhymchuk, A. 262 (1996) 33
Hendricks, J.H., see Tsukuda, T. 269 (1997) 17
Hendrickx, E., C. Boutton, K. Clays, A. Persoons, S. van Es, T. Biemans and B. Meijer, Quadratic nonlinear optical properties of correlated chromophores: cyclic 6,6′-dinitro-1,1′-binaphthyl-2,2′-ethers 270 (1997) 241
Henon, E., F. Bohr, A. Chakir and J. Brion, Theoretical study of the methyl peroxy self-reaction: the intermediate structure 264 (1997) 557
Herbich, J., A. Kapturkiewicz and J. Nowacki, Phosphorescent intramolecular charge transfer triplet states 262 (1996) 633
Herman, G.S., see Chambers, S.A. 267 (1997) 51
Herman, H., see Temsamani, M.A. 264 (1997) 556
Herman, M.F., see Lorenz, K.T. 261 (1996) 145
Herman, Z., see Wörgötter, R. 270 (1997) 333
Hernandez, M.I., see Buchachenko, A.A. 269 (1997) 448
Hernández-Trujillo, J., F. Colmenares, G. Cuevas and M. Costas, MP2 ab initio calculations of the hexafluorobenzene–benzene and –monofluorobenzene complexes 265 (1997) 503
Herrero, V.J., see Aoiz, F.J. 262 (1996) 175
Herrero, V.J., see Wrede, E. 265 (1997) 129
Herrero, V.J., see Aoiz, F.J. 264 (1997) 487
Herschbach, D., see Friedrich, B. 262 (1996) 41
Hertel, I.V., see Radloff, W. 261 (1996) 301
Hertel, I.V., see Freudenberg, Th. 269 (1997) 523
Hertel, I.V., see Radloff, W. 264 (1997) 210
Hertwig, R.H. and W. Koch, On the parameterization of the local correlation functional. What is Becke-3–LYP? 268 (1997) 345
Heseltine, T.H., see Ball, G.E. 261 (1996) 421
Heskett, D., see Andersen, J.N. 269 (1997) 371
Heskett, D., see McIlroy, D.N. 264 (1997) 168
Hess, W.P., see Rowland, B. 263 (1996) 574
Heufelder, J., H. Ruppe, S. Rutz, E. Schreiber and L. Wöste, Fractional revivals of vibrational wave packets in the NaK $A^1\Sigma^+$ state 269 (1997) 1
Heully, J.-L., see Reguero, M. 265 (1997) 621
Heydtmann, H., see Dehe, K. 262 (1996) 683
Heydtmann, H., see Jäger, M. 263 (1996) 817

Hidaka, M., T. Fujita, H. Nakai and H. Nakatsuji, Ab initio molecular orbital model of scanning tunneling microscopy. Benzene and benzene adsorbed on a Ag surface 264 (1997) 371
Hide, F., see Schwartz, B.J. 265 (1997) 327
Hildenbrand, D.L. and K.H. Lau, Dissociation energy of the molecule GeCl 263 (1996) 145
Hilger, R., H.-P. Merckens and H. Kleindienst, Accurate nonrelativistic energies for some doubly excited P^e states of He 262 (1996) 400
Hillenkamp, M., see Brownsword, R.A. 266 (1997) 259
Hillier, I.H., see Akhmatskaya, E.V. 267 (1997) 105
Hillier, I.H., see Andrews, S.B. 261 (1996) 521
Hillier, I.H., see Andrews, S.B. 269 (1997) 475
Hilt, O. and L.D.A. Siebbeles, Time and frequency dependent charge carrier mobility of one-dimensional chains with energetic disorder 269 (1997) 257
Hirano, M., see Judai, K. 270 (1997) 23
Hirao, K., see Kawashima, Y. 267 (1997) 82
Hirao, K., see Tsuneda, T. 268 (1997) 510
Hiraoka, K., J. Katsuragawa and A. Minamitsu, Thermochemistry of the $SiH_3^+ (SiH_4)_n$ and $SiH_3^+ (H_2)_n$ cluster ions 267 (1997) 580
Hirata, S., H. Torii, Y. Furukawa, M. Tasumi and J. Tomkinson, Inelastic neutron scattering from trans-polyacetylene 261 (1996) 241
Hirata, Y., see Katoh, R. 264 (1997) 631
Hirayama, S., see Niikura, H. 266 (1997) 217
Hirose, C., see Fujino, T. 261 (1996) 534
Hirose, T., see Uchimaru, T. 263 (1996) 691
Hirst, D.M., see Kim, G.-S. 264 (1997) 134
Hitchcock, A.P., see Kosugi, N. 265 (1997) 490
Ho, T.-I., see Wang, S.-L. 268 (1997) 434
Hoatson, G.L., see Vold, R.L. 263 (1996) 271
Hobza, P. and J. Šponer, Thermodynamic characteristics for the formation of H-bonded DNA base pairs 261 (1996) 379
Hobza, P., see Šponer, J. 267 (1997) 263
Hochstrasser, R.M., see Haran, G. 261 (1996) 389
Hochstrasser, R.M., see Kumble, R. 261 (1996) 396
Hodošček, M., see Kokalj, A. 268 (1997) 43
Hoff, A.J., see Spoyalov, A.P. 263 (1996) 715
Hoff, A.J., see Streltsov, A.M. 266 (1997) 347
Hoff, A.J., see Dzuba, S.A. 268 (1997) 273
Hoffman, B.M., see Doan, P.E. 269 (1997) 208
Hoffman, D.K., A. Frishman and D.J. Kouri, Distributed approximating functional approach to fitting multi-dimensional surfaces 262 (1996) 393
Hoffman, D.K., see Kouri, D.J. 262 (1996) 519
Hoffmann, S.K., see Tritt-Goc, J. 268 (1997) 471
Hofmann, G., see Fritzsche, S. 265 (1997) 253
Hohm, U., see Goebel, D. 265 (1997) 638
Holender, J.M., see Andrews, S.B. 261 (1996) 521
Holender, J.M., see Lindan, P.J.D. 261 (1996) 246
Holleman, I., see Warntjes, J.B.M. 261 (1996) 495
Holloway, J.H., see Cooke, S.A. 262 (1996) 308
Holloway, J.H., see Cooke, S.A. 266 (1997) 61

Holloway, J.H., see Evans, C.M. 267 (1997) 281
Holloway, J.H., see Cotti, G. 264 (1997) 513
Holmes, A.S., D.J.S. Birch, A. Sanderson and G.G. Aloisi, Time-resolved fluorescence photophysics of trans-stilbene in a DPPC lipid bilayer: evidence for a free rotation, location within two sites and a pre-liquid crystalline phase transition 266 (1997) 309
Holmes, J., see Gadd, G.E. 270 (1997) 108
Holmlid, L. and J. Wang, Electric field control of the rapid diffusion of K atoms into a graphite surface 268 (1997) 285
Holroyd, R.A., K. Itoh and M. Nishikawa, Studies of $e^- + CO_2 \rightleftharpoons CO_2^-$ equilibria in hexamethyldisiloxane and bis(trimethylsilyl)methane 266 (1997) 227
Holtz, M., see Sengupta, A. 263 (1996) 25
Hong, S.D. and M.S. Jhon, Restricted random search method based on taboo search in the multiple minima problem 267 (1997) 422
Hoogers, G. and D.A. King, A general theory for phase change kinetics with universal growth exponents 267 (1997) 37
Hori, M., see Yamazaki, T. 265 (1997) 137
Horváth, D., see Yamazaki, T. 265 (1997) 137
Hosoito, N., see Ueda, K. 261 (1996) 295
Hosokoshi, Y., see Deumal, M. 265 (1997) 190
Hou, X.-W., see Xie, M. 262 (1996) 1
Houben, L., see Smets, J. 262 (1996) 789
House, P.G. and E. Weitz, Reactions of molecular nitrogen and triethylamine with coordinatively unsaturated iron carbonyls: spin effects on reactions 266 (1997) 239
Howard, S.T., J.P. Foreman and P.G. Edwards, Correlated proton affinities of arylphosphines 264 (1997) 454
Howells, W.S., see Walters, J.K. 264 (1997) 539
Hrbek, J., S.Y. Li, J.A. Rodriguez, D.G. van Campen, H.H. Huang and G.-Q. Xu, Synthesis of sulfur films from S_2 gas: spectroscopic evidence for the formation of S_n species 267 (1997) 65
Hsiao, C.-C., see Kumar, A. 269 (1997) 22
Hsu, W.K., M. Terrones, J.P. Hare, H. Terrones, H.W. Kroto and D.R.M. Walton, Electrolytic formation of carbon nanostructures 262 (1996) 161
Hu, C.-H. and D.P. Chong, Density functional calculation of core-electron binding energies of transition metal carbonyl and nitrosyl complexes 262 (1996) 733
Hu, C.-H. and D.P. Chong, Density functional computations for inner-shell excitation spectroscopy 262 (1996) 729
Hu, J., see Zheng, G. 266 (1997) 533
Hua, Y., see Zhu, G. 264 (1997) 424
Huang, F.Q., see Tang, A.C. 263 (1996) 733
Huang, H.H., K.N. Fan, W. Huang, Z.H. Li, C.Y. Mok, W.N. Wang and W.S. Chin, An ab initio study on the thermal decomposition of γ-thiobutyrolactone 265 (1997) 508
Huang, H.H., see Hrbek, J. 267 (1997) 65
Huang, J.-S., see Cheng, W.-D. 261 (1996) 66
Huang, J.Q., see Urban, J. 264 (1997) 441
Huang, K.L., see Liou, H.T. 266 (1997) 591
Huang, S., see Zhang, J. 268 (1997) 449
Huang, W., see Huang, H.H. 265 (1997) 508
Huang, X., see Ge, M. 264 (1997) 139

Huang, X.-Z., see Lin, L.-R. 266 (1997) 358
Huang, X.-Z., see Du, X.-Z. 268 (1997) 31
Huang, Y. and R. Liu, Investigation of the change in band structure of a carbon nanotube due to a distortion keeping the initial translational symmetry 268 (1997) 365
Huang, Z., see Zhao, L. 263 (1996) 235
Huber, G., see Hazenkamp, M.F. 265 (1997) 264
Huber, H., B. Kirchner, J. Solca and G. Steinebrunner, An unusual basis set superposition error in the electric field gradient of the neon dimer calculated with bond functions 266 (1997) 388
Huber, J.R., see Gejo, T. 261 (1996) 443
Hudgens, J.W., see Ashfold, M.N.R. 263 (1996) 138
Hudgens, J.W., see Johnson III, R.D. 261 (1996) 474
Hudgins, R.R., see Dugourd, P. 267 (1997) 186
Hudson, E.A., see Moler, E.J. 264 (1997) 502
Huet, T.R., see Hadj Bachir, I. 270 (1997) 533
Huff, W.R.A., see Moler, E.J. 264 (1997) 502
Hughes, J.M., see Smart, B. 261 (1996) 51
Huisken, F., M. Kaloudis and A.A. Vigasin, Vibrational frequency shifts caused by weak intermolecular interactions 269 (1997) 235
Hull, W.E., see Gromov, A. 267 (1997) 460
Hulsebosch, R.J., see Spoyalov, A.P. 263 (1996) 715
Hung, W.-C., see Kumar, A. 269 (1997) 22
Hunter, M., see Talukdar, R.K. 262 (1996) 669
Huppert, D., see Zolotov, B. 265 (1997) 418
Hurwood, D.J., see Gadd, G.E. 261 (1996) 221
Hurwood, D.J., see Gadd, G.E. 270 (1997) 108
Husain, D., see Fernández, J.A. 267 (1997) 301
Hussain, Z., see Moler, E.J. 264 (1997) 502
Hutter, J., see Haase, F. 266 (1997) 397
Hvelplund, P., see Shen, H. 264 (1997) 508
Hynes, A.J., see Silvente, E. 264 (1997) 309
Hynninen, P.H., see Tkachenko, N.V. 261 (1996) 234
Hyvönen, M., M. Ala-Korpela, J. Vaara, T.T. Rantala and J. Jokisaari, Inequivalence of single CH_a and CH_b methylene bonds in the interior of a diunsaturated lipid bilayer from a molecular dynamics simulation 268 (1997) 55

Iannotta, S., see Biasioli, F. 270 (1997) 115
Ibuki, K., see Hamanoue, K. 267 (1997) 165
Ibuki, T. and K. Okada, Photoabsorption and fluorescence excitation spectra of CF_3CN in the region of 6–41 eV 263 (1996) 173
Ichimura, T., see Suzuki, T. 263 (1996) 197
Ichimura, T., see Suzuki, T. 266 (1997) 107
Iglesias-Groth, S., J. Breton and C. Girardet, An analytical approach for the interlayer interaction in spherical buckyonions 264 (1997) 351
Iijima, S., see Qin, L.-C. 262 (1996) 252
Iijima, S., see Qin, L.-C. 268 (1997) 101
Iijima, S., see Qin, L.-C. 269 (1997) 65
Ikeda, N., see Islam, A. 263 (1996) 209
Ikeguchi, M., see Shimizu, S. 268 (1997) 93

Ilangovan, U. and P. Raghunathan, EPR lineshapes and dynamics of TEMPOL solubilized in the aqueous microphase of lecithin/cyclohexane/water reverse micelles 263 (1996) 223
Illenberger, E., see Matejcik, S. 261 (1996) 437
Illenberger, E., see Matejcik, S. 267 (1997) 329
Illingworth, R., see Qi, X. 264 (1997) 623
Imahori, H., K. Hagiwara, T. Akiyama, M. Aoki, S. Taniguchi, T. Okada, M. Shirakawa and Y. Sakata, The small reorganization energy of C_{60} in electron transfer 263 (1996) 545
Imahori, H., see Zhao, X. 262 (1996) 643
Imajo, T., see Ishiguro, M. 263 (1996) 629
Imamoto, Y., see Chosrowjan, H. 270 (1997) 267
Imamura, T., see Rudich, Y. 261 (1996) 467
Imans, F., L. Viaene, M. Van der Auweraer and F.C. De Schryver, Local properties of adsorption sites probed by the emission of fluorophores of different size and shape 262 (1996) 583
Imhof, R., H. Teramae and J. Michl, Conformational effects in UV absorption spectra of tetrasilanes 270 (1997) 500
Infante, G., see Polzonetti, G. 267 (1997) 384
Inokuchi, Y., Y. Naitoh, K. Ohashi, K.-i. Saitow, K. Yoshihara and N. Nishi, Formation of benzene dimer cations in neat liquid benzene studied by femtosecond transient absorption spectroscopy 269 (1997) 298
Inokuchi, Y., see Ohashi, K. 263 (1996) 167
Inoue, Y., see Kohno, M. 267 (1997) 72
Inoue, Y., see Yamanaka, T. 264 (1997) 180
Irie, M., see Miyasaka, H. 269 (1997) 281
Ishchenko, V.N., see Makarov, V.I. 266 (1997) 303
Ishibashi, T. and H. Hamaguchi, The central CC bond stretch frequencies and structure of S_2 and S_1 diphenylacetylene in solution studied by picosecond time-resolved CARS spectroscopy 264 (1997) 551
Ishida, T., see Murai, H. 264 (1997) 619
Ishiguro, M., T. Imajo, K. Harada, M. Matsubara, K. Tanaka and T. Tanaka, New discharge modulation technique for detection of transient species produced in pulsed supersonic jet by color center laser spectroscopy 263 (1996) 629
Ishikawa, K., see Pola, J. 262 (1996) 279
Ishikawa, M., see Kamiya, N. 265 (1997) 595
Ishikawa, T., see Yamazaki, T. 265 (1997) 137
Ishikawa, Y., see Koc, K. 263 (1996) 338
Ishiwata, T., Y. Kasai and K. Obi, Observation of the $0_u^-(^3P_1)$ ion-pair state of Cl_2 by perturbation-facilitated optical–optical double resonance 261 (1996) 175
Ishiwata, T., see Wheeler, M.D. 268 (1997) 421
Islam, A., N. Ikeda, K. Nozaki and T. Ohno, Role of higher excited states in radiative and nonradiative processes of coordination compounds of Ru(II) and Rh(III) in crystal 263 (1996) 209
Itaya, A., see Kotani, S. 269 (1997) 274
Itaya, A., see Miyasaka, H. 269 (1997) 281
Ithnin, R., see Jones, R.G. 261 (1996) 539
Ito, F., see Nakanaga, T. 261 (1996) 414
Ito, F., see Nakanaga, T. 267 (1997) 491
Ito, M., see Song, M.-B. 263 (1996) 585
Itoh, C., T. Kondoh and K. Tanimura, Time-resolved spectroscopic study of the initial process of photopolymerization in a diacetylene crystal 261 (1996) 191

Itoh, K., see Holroyd, R.A. 266 (1997) 227
Itoh, K., see Teki, Y. 270 (1997) 573
Itoh, S., see Dzuba, S.A. 264 (1997) 238
Iucci, G., see Polzonetti, G. 267 (1997) 384
Ivanov, M.Yu. and A. Stolow, Coherent control of high-n Rydberg lifetimes using wavepacket technology 265 (1997) 231
Iwaki, M., see Dzuba, S.A. 264 (1997) 238
Iwasaki, Y., see Murai, H. 264 (1997) 619
Iwata, K. and H.-o. Hamaguchi, Temperature dependent kinetics of the picosecond bimolecular reaction between S_1 trans-stilbene and carbon tetrachloride: is the ultrafast photochemical reaction diffusion-controlled? 261 (1996) 208
Izvekov, V., see Macsári, I. 269 (1997) 393

Jackson, B., Reduced density matrix approach for gas–solid scattering 270 (1997) 484
Jackson, G., see Gil-Villegas, A. 269 (1997) 441
Jackson, K.A., see Rencsok, R. 262 (1996) 207
Jacobi, K., see Schwegmann, S. 264 (1997) 680
Jäger, M., H. Heydtmann and C. Zetzsch, Vacuum ultraviolet spectrum and quantum yield of the 193 nm photolysis of phosgene 263 (1996) 817
Jäger, W., S. Schneider and J.W. Verhoeven, Influence of solvent viscosity and permittivity on the harpooning mechanism in semirigidly bridged electron donor–acceptor systems 270 (1997) 50
Jakob, P., Identification of a surface reaction product by detection of a vibrational combination band 263 (1996) 607
Jakubek, Z.J. and M. Takami, Ab initio studies of AgHe exciplex 265 (1997) 653
James, M., see Gadd, G.E. 261 (1996) 221
Jang, J.H., see Kim, K.S. 265 (1997) 497
Janik-Czachor, M., see Bukowska, J. 268 (1997) 481
Janke, W. and T. Sauer, Multigrid method versus staging algorithm 263 (1996) 488
Janssen, M.H.M., see Biesheuvel, C.A. 269 (1997) 515
Jardon, P., see Arabei, S.M. 270 (1997) 31
Jarrold, M.F., see Dugourd, P. 267 (1997) 186
Jarrold, M.F., see Shvartsburg, A.A. 261 (1996) 86
Jayathirtha Rao, V., see Raj Gopal, V. 270 (1997) 593
Jeffreys, N., I.W. Griffiths, D.E. Parry and F.M. Harris, A combined computational and experimental study of the triple ionization of carbon disulphide 266 (1997) 537
Jeffreys, N., see Silcocks, S.E. 262 (1996) 355
Jegerschöld, C., see Deligiannakis, Y. 270 (1997) 564
Jenniskens, H.G., W. van Essenberg, M. Kadodwala and A.W. Kleyn, The photodissociation of tert-butyl nitrite adsorbed on Ag(111): bimodal velocity distributions of the photoproducts 268 (1997) 7
Jensen, F., The magnitude of intramolecular basis set superposition error 261 (1996) 633
Jeon, S.-J., see Song, N.W. 261 (1996) 307
Jeong, H.Y. and Y.-K. Han, Comment on ''A computational study of the structures of van der Waals and hydrogen-bonded complexes of ethene and ethyne'' 263 (1996) 345
Jeoung, S.C., see Song, N.W. 261 (1996) 307
Jesse, K.J., Structural impacts on the photodissociation dynamics of aromatic endoperoxides in solution 264 (1997) 193
Jeziorski, B., see Williams, H.L. 262 (1996) 431

Jhon, M.S., see Hong, S.D. 267 (1997) 422
Jiang, Y., The interaction between two charged plates in electrolyte solutions 263 (1996) 317
Jiang, Y.-B., see Lin, L.-R. 266 (1997) 358
Jiang, Y.-B., see Du, X.-Z. 268 (1997) 31
Jiao, C.Q., R. Nagpal and P. Haaland, Ion chemistry in boron trichloride BCl_3 265 (1997) 239
Jiao, C.Q., R. Nagpal and P.D. Haaland, Ion chemistry in trifluoromethane, CHF_3 269 (1997) 117
Joachim, C. and J.K. Gimzewski, An electromechanical amplifier using a single molecule 265 (1997) 353
Jodl, H.J., see Gellini, C. 268 (1997) 381
Joens, J.A., Alternative assignments for the vibrational structure of the $^3B_1$–$X\,^1A_1$ band system of SO_2 261 (1996) 659
Johannes, H.-H., see Werncke, W. 266 (1997) 99
Johnsen, R., see Gougousi, T. 265 (1997) 399
Johnson, C.K., see Larson, E.J. 265 (1997) 161
Johnson, M.A., see Bailey, C.G. 265 (1997) 185
Johnson, M.A., see Bailey, C.G. 269 (1997) 122
Johnson, M.A., see Tsukuda, T. 268 (1997) 429
Johnson, M.A., see Tsukuda, T. 269 (1997) 17
Johnson, P., see Gadd, G.E. 270 (1997) 108
Johnson III, R.D., J.W. Hudgens and M.N.R. Ashfold, Excited electronic states of the SiF_2 radical studied by resonance enhanced multiphoton ionisation spectroscopy and by ab initio methods 261 (1996) 474
Johnson III, R.D., see Ashfold, M.N.R. 263 (1996) 138
Jokisaari, J., see Koskela, T. 261 (1996) 425
Jokisaari, J., see Hyvönen, M. 268 (1997) 55
Jonah, C.D., see Zhang, X. 262 (1996) 649
Jonah, C.D., see Takahashi, K. 264 (1997) 297
Jones, M.R., see Van Brederode, M.E. 268 (1997) 143
Jones, R.G., S. Turton and R. Ithnin, Formation of translationally hot ethene by dissociative electron capture of adsorbed 1,2-dichloroethane 261 (1996) 539
Jongma, R.T., G. von Helden, G. Berden and G. Meijer, Confining CO molecules in stable orbits 270 (1997) 304
Jonsson, D., see Norman, P. 268 (1997) 337
Joos, S., see Albert, G. 268 (1997) 235
Jorge, F.E., T.B. Bobbio and A.B.F. da Silva, Adapted Gaussian basis sets for the relativistic closed-shell atoms from helium to barium generated with the generator coordinate Dirac–Fock method 263 (1996) 775
Jørgensen, P., see Christiansen, O. 261 (1996) 369
Jørgensen, P., see Christiansen, O. 263 (1996) 530
Jørgensen, P., see Hättig, C. 269 (1997) 428
Jouvet, C., see Dedonder-Lardeux, C. 264 (1997) 596
Judai, K., M. Hirano, H. Kawamata, S. Yabushita, A. Nakajima and K. Kaya, Formation of vanadium–arene complex anions and their photoelectron spectroscopy 270 (1997) 23
Jung, K.-H., see Kim, D.-C. 265 (1997) 573
Jungkamp, T.P.W. and J.H. Seinfeld, The mechanism of methoxy radical oxidation: hydrogen abstraction versus trioxy radical formation 263 (1996) 371
Jursic, B.S., Ab initio and density functional theory study of the diazene isomerization 261 (1996) 13
Jursic, B.S., Exploring the potential energy surface of the hydrogen abstraction reaction from hydrochloric acid with hydrogen and methyl radicals using ab initio and density functional theory methods. An example of a polar radical hydrogen abstraction reaction 264 (1997) 113

Ka, J. and S. Shin, Dynamics of molecular ion (I_2^-) in condensed phases: hybrid quantum/classical method for a linear chain model 269 (1997) 227
Kachanov, A.A., see Romanini, D. 270 (1997) 538
Kachanov, A.A., see Romanini, D. 270 (1997) 546
Kachanov, A.A., see Romanini, D. 264 (1997) 316
Kaczmarek, Ł., see Grabowska, A. 267 (1997) 132
Kadodwala, M., see Jenniskens, H.G. 268 (1997) 7
Kadyshevitch, A., see Haran, A. 268 (1997) 475
Kagawa, T., see Koc, K. 263 (1996) 338
Kahn-Harari, A., see Agafonov, V. 267 (1997) 193
Kahn, O., Competing spin interactions and degenerate frustration for discrete molecular species 265 (1997) 109
Kai, Y., see Ueda, K. 261 (1996) 295
Kajimoto, O., see Fujiwara, T. 261 (1996) 201
Kajimoto, O., see Lee, S. 265 (1997) 579
Kalb, M., see Gudipati, M.S. 268 (1997) 169
Kalinin, S.V., see Vertegel, A.A. 262 (1996) 455
Kalinowski, J., G. Giro, P. Di Marco, N. Camaioni and V. Fattori, Exciton dynamics in an aromatic diamine at the interface with 8-hydroxyquinoline aluminum 265 (1997) 607
Kalmus, P., see McCarthy, M.C. 264 (1997) 252
Kalnin, Yu.R.H., G.J. Zvejnieks and E.A. Kotomin, The effect of the particle generation function on the rate of the diffusion-controlled $A + B \rightarrow B$ reaction with a permanent particle source 270 (1997) 229
Kaloudis, M., see Huisken, F. 269 (1997) 235
Kalyanaraman, C., see Chakrabarti, N. 267 (1997) 31
Kamada, K., M. Ueda, T. Sakaguchi, K. Ohta and T. Fukumi, Femtosecond optical Kerr study of heavy atom effects on the third-order optical nonlinearity of thiophene homologues: purely electronic contribution (Chem. Phys. Letters 263 (1996) 215). Erratum 267 (1997) 402
Kamada, K., M. Ueda, T. Sakaguchi, K. Ohta and T. Fukumi, Femtosecond optical Kerr study of heavy atom effects on the third-order optical nonlinearity of thiophene homologues: purely electronic contribution 263 (1996) 215
Kamata, Y., see Maeda, K. 262 (1996) 110
Kambanis, K.G., Y.G. Lazarou and P. Papagiannakopoulos, Gas phase reaction kinetics of Cl atoms with ICH_2OCH_3 261 (1996) 457
Kambanis, K.G., Y.G. Lazarou and P. Papagiannakopoulos, Absolute reaction rate of chlorine atoms with iodomethane 268 (1997) 498
Kamimoto, T., see Hashimoto, K. 266 (1997) 7
Kamiya, N., M. Ishikawa, K. Kasahara, M. Kaneko, N. Yamamoto and H. Ohtani, Picosecond fluorescence spectroscopy of the purple membrane of *Halobacterium halobium* in alkaline suspension 265 (1997) 595
Kammler, Th. and J. Küppers, Methanation of carbon on Ni(100) surfaces at 120 K with gaseous H atoms 267 (1997) 391
Kanayama, K., see Koga, T. 266 (1997) 123
Kandel, S.A., T.P. Rakitzis, T. Lev-On and R.N. Zare, Dynamical effects of reagent vibrational excitation in the $Cl + C_2H_6(\nu_5 = 1) \rightarrow HCl + C_2H_5$ reaction 265 (1997) 121
Kanehisa, N., see Ueda, K. 261 (1996) 295

Kaneko, H., M. Hada, T. Nakajima and H. Nakatsuji, Spin–orbit effect on the magnetic shielding constant using the ab initio UHF method: tin tetrahalides 261 (1996) 1
Kaneko, H., see Hada, M. 261 (1996) 7
Kaneko, M., see Kamiya, N. 265 (1997) 595
Kaneti, J., see Siebrand, W. 266 (1997) 47
Kang, H.C., Reply to Comment on "A computational study of the structures of van der Waals and hydrogen-bonded complexes of ethene and ethyne" 263 (1996) 348
Kang, T.-I., see Song, N.W. 261 (1996) 307
Kanhere, D.G., see Majumder, C. 261 (1996) 515
Kanik, I., see Trajmar, S. 262 (1996) 241
Kanno, H., see Ohnishi, A. 263 (1996) 259
Kano, S.S., see Fujino, T. 261 (1996) 534
Kaplan, T.A., see Rencsok, R. 262 (1996) 207
Kappes, M.M., see Cummins, T.R. 261 (1996) 228
Kapturkiewicz, A., see Herbich, J. 262 (1996) 633
Karasiev, V., see López-Boada, R. 270 (1997) 443
Kärger, J., see Fritzsche, S. 265 (1997) 253
Karlsson, L., see Doverstål, M. 270 (1997) 273
Karlström, G., see Engkvist, O. 265 (1997) 19
Karpiuk, J., see Grabowska, A. 267 (1997) 132
Karplus, M., see Neria, E. 267 (1997) 23
Kasahara, K., see Kamiya, N. 265 (1997) 595
Kasai, T., see Takahashi, H. 264 (1997) 44
Kasai, Y., see Ishiwata, T. 261 (1996) 175
Kasemo, B., see Åkerlund, C. 270 (1997) 157
Kasha, M., see Carlos del Valle, J. 263 (1996) 154
Kashevarova, L.S., see Agafonov, V. 267 (1997) 193
Kashitani, M., see Fujino, T. 261 (1996) 534
Kashtanov, S.A., see Aleinikov, N.N. 267 (1997) 155
Kassab, E., see Šepa, J. 262 (1996) 321
Kataura, H., see Qin, L.-C. 268 (1997) 101
Katayama, S., see Egawa, C. 266 (1997) 169
Katheder, I., see Limantara, L. 262 (1996) 656
Katoh, R., M. Kotani, Y. Hirata and T. Okada, Triplet exciton formation in a benzophenone single crystal studied by picosecond time-resolved absorption spectroscopy 264 (1997) 631
Katsuragawa, J., see Hiraoka, K. 267 (1997) 580
Kauffmann, E., H. Frei and R.A. Mathies, Nanosecond time-resolved step-scan FT-IR spectroscopy of the photochemical ring-opening of 1,3-cyclohexadiene 266 (1997) 554
Kaupp, M., O.L. Malkina and V.G. Malkin, Interpretation of ^{13}C NMR chemical shifts in halomethyl cations. On the importance of spin–orbit coupling and electron correlation 265 (1997) 55
Kawai, A., see Mitsui, M. 262 (1996) 125
Kawai, T., see Tokue, I. 270 (1997) 587
Kawakami, T., S. Takeda, W. Mori and K. Yamaguchi, Theoretical study of the effective exchange interactions between nitroxides via hydrogen atoms 261 (1996) 129
Kawamata, H., see Judai, K. 270 (1997) 23
Kawamata, H., see Negishi, Y. 269 (1997) 199
Kawamata, K., see Nakanaga, T. 267 (1997) 491
Kawamori, A., see Dzuba, S.A. 264 (1997) 238

Kawashima, Y., K. Nakayama, H. Nakano and K. Hirao, Theoretical study of the $\pi \rightarrow \pi^*$ excited states of linear polyene radical cations and dications 267 (1997) 82
Kaya, K., see Judai, K. 270 (1997) 23
Kaya, K., see Negishi, Y. 269 (1997) 199
Kellar, S.A., see Moler, E.J. 264 (1997) 502
Keller, R.A., see Enderlein, J. 270 (1997) 464
Keller, R.A., see Ambrose, W.P. 269 (1997) 365
Kennedy, S., see Gadd, G.E. 261 (1996) 221
Kern, K., see Cavalleri, O. 269 (1997) 479
Kertesz, M., see Choi, C.H. 263 (1996) 697
Kettler, M., see Vörtler, H.L. 266 (1997) 368
Ketzer, B., see Yamazaki, T. 265 (1997) 137
Khairallah, G. and J.B. Peel, Identification of cyano dianions of C_{60} by electrospray mass spectrometry 268 (1997) 218
Khalil, B., O. Cisse, G. Moreau, F. Thibault, R. Le Doucen and J. Boissoles, Line mixing and line broadening in CO_2 bands perturbed by helium at 193 K 263 (1996) 811
Khan, A., R. Khan, M.F. Khan and F. Khanam, A cluster model explaining quantitatively the anomalous variation of density of water with temperature 266 (1997) 473
Khan, M.A., R.A. Qureshi and M.A. Gondal, Ar-supported atomic population transfer from the $3d4p\ ^1D_2$ to nearby states of Ca 264 (1997) 273
Khan, M.F., see Khan, A. 266 (1997) 473
Khan, R., see Khan, A. 266 (1997) 473
Khanam, F., see Khan, A. 266 (1997) 473
Khanna, S.N., see Reuse, F.A. 267 (1997) 258
Khidekel, V. and S. Mukamel, High-order echoes in vibrational spectroscopy of liquids (Chem. Phys. Letters 240 (1995) 304). Erratum 263 (1996) 350
Khoury, J.T., see Alvarez, M.M. 266 (1997) 91
Kidd, R.T., S.R. Meech and D. Lennon, Enhanced photodesorption of NO on roughened silver surfaces 262 (1996) 142
Kido, G., see Nishizawa, K. 267 (1997) 501
Kidoaki, S., see Noguchi, H. 261 (1996) 527
Kiefer, B., see Bañares, L. 267 (1997) 141
Kiefer, W., see Schmitt, M. 270 (1997) 9
Kiefer, W., see Trunk, M. 264 (1997) 233
Kiendler, A., see Matejcik, S. 261 (1996) 437
Kiendler, A., see Matejcik, S. 267 (1997) 329
Kim, D., see Song, N.W. 261 (1996) 307
Kim, D., see Kim, Y. 264 (1997) 673
Kim, D.-C., J.W. Hahn, E.S. Lee and K.-H. Jung, Photodissociation dynamics of H_2S at 266 nm via the degenerate four-wave mixing spectroscopy 265 (1997) 573
Kim, G.-S. and D.M. Hirst, Ab initio potential-energy curves for excited electronic states of the molecular ion $AsCl^+$ 264 (1997) 134
Kim, G.H., see Bae, S.C. 265 (1997) 385
Kim, H.S., see Fujii, T. 268 (1997) 229
Kim, J., see Kim, K.S. 265 (1997) 497
Kim, J., see Bailey, C.G. 269 (1997) 122
Kim, J.U., W.K. Hartmann, H.J. Schock, B. Golding and D.G. Nocera, The electron donor–acceptor exciplex of N,N-dimethylaniline and 1,4,6-trimethylnaphthalene 267 (1997) 323

Kim, K.S., J.Y. Lee, H.S. Choi, J. Kim and J.H. Jang, Quantum mechanical probabilistic structure of the benzene–water complex 265 (1997) 497
Kim, M.S., see Lee, T.G. 264 (1997) 303
Kim, S.G., Y.H. Lee, P. Nordlander and D. Tománek, Disintegration of finite carbon chains in electric fields 264 (1997) 345
Kim, S.G., see Lee, Y.H. 265 (1997) 667
Kim, S.G., see Grönbeck, H. 264 (1997) 39
Kim, Y., H.W. Cheon, M. Yoon, N.W. Song and D. Kim, SiO_2 colloidal effects on the twisted intramolecular charge transfer of *p*-N,N-dimethylaminobenzoic acid in acetonitrile 264 (1997) 673
Kim, Y.-K., see Koc, K. 263 (1996) 338
Kim, Y.J., see Chambers, S.A. 267 (1997) 51
Kimura, K., see Vondrák, T. 261 (1996) 481
Kimura, M., see Dutta, C.M. 264 (1997) 51
Kimura, Y., see Umemoto, H. 264 (1997) 215
King, A., see Hayden, B.E. 269 (1997) 485
King, D.A., see Hoogers, G. 267 (1997) 37
Kinoshita, M., see Deumal, M. 265 (1997) 190
Kirchner, B., see Huber, H. 266 (1997) 388
Kiribayashi, S., see Nakano, M. 262 (1996) 66
Kiribayashi, S., see Yamada, S. 267 (1997) 438
Kiribayashi, S., see Yamada, S. 267 (1997) 445
Kirtman, B. and H. Sekino, Local quantum chemistry. Incorporation of pseudospectral methodology into the local space approximation 263 (1996) 313
Kishi, R., see Negishi, Y. 269 (1997) 199
Kiskinova, M., see Comelli, G. 261 (1996) 253
Kitagawa, T., see Kruglik, S.G. 266 (1997) 283
Kitagawa, T., see Verma, A.L. 267 (1997) 507
Kitagawa, T., see Zhao, X. 262 (1996) 643
Kitahama, Y. and H. Murai, CIDEP study on the flash photolysis of benzoin included in β-cyclodextrin 261 (1996) 160
Kiwi, J., see Vuissoz, P.-A. 264 (1997) 366
Klein, U.K.A., see Than Htun, M. 264 (1997) 285
Kleindienst, H., see Hilger, R. 262 (1996) 400
Kleindienst, H., see Barrois, R. 268 (1997) 531
Kleinermanns, K., see Schumm, S. 263 (1996) 126
Kleinke, M.U., see Kubota, L.T. 264 (1997) 662
Kleyn, A.W., see Jenniskens, H.G. 268 (1997) 7
Klinowski, J., see Cheng, C.-F. 263 (1996) 247
Klinowski, J., see Kolodziejski, W. 266 (1997) 597
Klinowski, J., see Lee, M.-H. 265 (1997) 673
Klopper, W. and H.P. Lüthi, Towards the accurate computation of properties of transition metal compounds: the binding energy of ferrocene 262 (1996) 546
Klopper, W., M. Quack and M.A. Suhm, A new ab initio based six-dimensional semi-empirical pair interaction potential for HF 261 (1996) 35
Klopper, W., see Tunega, D. 269 (1997) 435
Knickelbein, M.B., see Koretsky, G.M. 267 (1997) 485
Knight, A.M., see Stangassinger, A. 266 (1997) 189

Knippels, G.M.H., see Engeln, R. 269 (1997) 293
Knopp, G., see Schmitt, M. 270 (1997) 9
Knor, Z., see Mingo, N. 263 (1996) 8
Knowles, P.J., see Mura, M.E. 262 (1996) 533
Knowles, P.J., see Tuckett, R.P. 261 (1996) 486
Ko, D.-S., M. Sauer, S. Nord, R. Müller and J. Wolfrum, Determination of the diffusion coefficient of dye in solution at single molecule level 269 (1997) 54
Ko, D.-S., see Müller, R. 262 (1996) 716
Kobayashi, K. and S. Nagase, Structures and electronic states of endohedral dimetallofullerenes: $M_2@C_{80}$ (M = Sc, Y, La, Ce, Pr, Eu, Gd, Yb and Lu) 262 (1996) 227
Kobayashi, K., S. Nagase and T. Akasaka, Endohedral dimetallofullerenes $Sc_2@C_{84}$ and $La_2@C_{80}$. Are the metal atoms still inside the fullerene cages? 261 (1996) 502
Kobayashi, K., see Suzuki, Y. 268 (1997) 213
Kobayashi, R. and A.P. Rendell, A direct coupled cluster algorithm for massively parallel computers 265 (1997) 1
Kobayashi, T., M. Yasuda, S. Okada, H. Matsuda and H. Nakanishi, Femtosecond spectroscopy of a polydiacetylene with extended conjugation to acetylenic side groups 267 (1997) 472
Kobayashi, T., see Geng, J. 266 (1997) 290
Kobayashi, T., see Qiu, F. 266 (1997) 153
Kobayashi, T., see Teki, Y. 270 (1997) 573
Kobori, Y., see Mitsui, M. 262 (1996) 125
Kobryanskii, V.M., see Frankevich, E.L. 261 (1996) 545
Koc, K., Y. Ishikawa, T. Kagawa and Y.-K. Kim, Relativistic modification of asymptotic configuration interaction in the carbon isoelectronic sequence 263 (1996) 338
Koch, H., see Christiansen, O. 261 (1996) 369
Koch, H., see Christiansen, O. 263 (1996) 530
Koch, H., see Hättig, C. 269 (1997) 428
Koch, W., see Hertwig, R.H. 268 (1997) 345
Kochubei, S.A., see Makarov, V.I. 266 (1997) 303
Kodaka, T., see Harima, Y. 267 (1997) 481
Koga, T. and K. Kanayama, Noninteger principal quantum numbers increase the efficiency of Slater-type basis sets: heavy atoms 266 (1997) 123
Koga, Y., see Pola, J. 262 (1996) 279
Kogej, T., see Cross, G.H. 268 (1997) 36
Kohama, M., see Ueda, K. 261 (1996) 295
Kohn, S.C., see Dirken, P.J. 266 (1997) 568
Kohno, M., S. Ogura, K. Sato and Y. Inoue, Properties of photocatalysts with tunnel structures: formation of a surface lattice O^- radical by the UV irradiation of $BaTi_4O_9$ with a pentagonal-prism tunnel structure 267 (1997) 72
Koivusaari, M., see Ulenikov, O.N. 268 (1997) 242
Kokalj, A., A. Lesar and M. Hodošček, Interaction of oxygen with the Pt(111) surface: a cluster model study 268 (1997) 43
Koll, A., see Rospenk, M. 261 (1996) 283
Kollmar, C., A new concept for an approximate MO formalism 269 (1997) 215
Kolodziejski, W. and J. Klinowski, $^{31}P \rightarrow {}^{1}H$ cross-polarization and ^{1}H spin diffusion NMR in the large-pore gallophosphate molecular sieve cloverite 266 (1997) 597
Komaguchi, K., M. Shiotani and A. Lund, An ESR study of trimethylenemethane radical cation 265 (1997) 217

Komaguchi, K., T. Kumada, Y. Aratono and T. Miyazaki, Evaluation of the distance between the hydrogen atom and hydrogen molecule in the tunneling reaction HD + D → H + D_2 in an argon matrix at 20 K 268 (1997) 493
Komaguchi, K., see Kumada, T. 261 (1996) 463
Komatsuzaki, T. and M. Nagaoka, A dividing surface free from a barrier recrossing motion in many-body systems 265 (1997) 91
Komorowski, L., see Lipiński, J. 262 (1996) 449
Kompa, K.L., see Fuß, W. 262 (1996) 675
Kondo, J.N., see Fujino, T. 261 (1996) 534
Kondoh, T., see Itoh, C. 261 (1996) 191
Kondow, T., see Terasaki, A. 262 (1996) 269
Kondow, T., see Tsukuda, T. 269 (1997) 17
Kong, M.J., S.S. Lee, J. Lyubovitsky and S.F. Bent, Infrared spectroscopy of methyl groups on silicon 263 (1996) 1
Konings, R.J.M., see Kovács, A. 268 (1997) 207
Kontoleta, P., see Georgiou, S. 270 (1997) 491
Koplitz, B., see Lorenz, K.T. 261 (1996) 145
Koput, J., The equilibrium structure and spectroscopic constants of HCP – an ab initio study 263 (1996) 401
Koretsky, G.M. and M.B. Knickelbein, Infrared photodissociation spectroscopy of $Ag_n(C_6H_6)_m$ and $Ag_n(C_6D_6)_m$ clusters: evidence of adsorption-induced symmetry reduction in benzene 267 (1997) 485
Korn, G., see Freudenberg, Th. 269 (1997) 523
Korona, T., see Williams, H.L. 262 (1996) 431
Koskela, T., M. Ylihautala, J. Vaara and J. Jokisaari, ^{13}C NMR spectroscopy of methane adsorbed in SAPO-11 molecular sieve 261 (1996) 425
Kosugi, N., R.G. Cavell and A.P. Hitchcock, (LS) versus (jj) coupling in P 2p inner-shell excited states of PF_3 265 (1997) 490
Kotani, M., see Katoh, R. 264 (1997) 631
Kotani, S., H. Miyasaka, A. Itaya, Y. Hamanaka, N. Mataga, S. Nakajima and A. Osuka, Picosecond dynamics of intramolecular charge-transfer processes of β-substituted porphyrins adsorbed on the porous glass 269 (1997) 274
Kotomin, E.A., see Kalnin, Yu.R.H. 270 (1997) 229
Kotterer, M. and J.P. Maier, Electronic spectrum of C_6H: $^2\Pi$–X $^2\Pi$ in the gas-phase detected by cavity ringdown 266 (1997) 342
Koubenakis, A., see Georgiou, S. 270 (1997) 491
Kouri, D.J., D.K. Hoffman, T. Peng and J.H.Z. Zhang, Reactant-product decoupling for state-to-state reactive scattering: further partitioning in the product arrangements 262 (1996) 519
Kouri, D.J., see Hoffman, D.K. 262 (1996) 393
Kovács, A., R.J.M. Konings and A.S. Booij, High-temperature infrared spectra of $LaCl_3$, $Labr_3$, and LaI_3 268 (1997) 207
Kovács, A., see Macsári, I. 269 (1997) 393
Kownacki, K., see Grabowska, A. 267 (1997) 132
Koyama, Y., see Limantara, L. 262 (1996) 656
Kozlova, S.G., see Gabuda, S.P. 263 (1996) 253
Kraka, E., D. Cremer, G. Bucher, H. Wandel and W. Sander, A CCSD(T) and DFT investigation of *m*-benzyne and 4-hydroxy-*m*-benzyne 268 (1997) 313
Krätschmer, W., see Gromov, A. 267 (1997) 460

Krempl, S., Properties of the path-class expansion in the continuous limit 263 (1996) 283
Kristóf, T. and J. Liszi, Alternative implementations of the Gibbs ensemble Monte Carlo calculation 261 (1996) 620
Kroon, A., see Baltuška, A. 270 (1997) 263
Kroto, H.W., see Hsu, W.K. 262 (1996) 161
Kruglik, S.G., V.V. Ermolenkov, A.G. Shvedko, V.A. Orlovich, V.A. Galievsky, V.S. Chirvony, C. Otto and P.-Y. Turpin, Intermolecular interaction of photoexcited Cu(TMpy-P4) with water studied by transient resonance Raman and picosecond absorption spectroscopies 270 (1997) 293
Kruglik, S.G., Y. Mizutani and T. Kitagawa, Time-resolved resonance Raman study of the primary photoprocesses of nickel(II) octaethylporphyrin in solution 266 (1997) 283
Krupa, J.-C., see Deren, P.J. 264 (1997) 614
Ku, J.K., see Bae, S.C. 265 (1997) 385
Ku, J.K., see Lee, K. 262 (1996) 610
Kubota, J., see Fujino, T. 261 (1996) 534
Kubota, L.T., M.U. Kleinke, C. Mello, M.I. Bueno and G. de Oliveira Neto, Experimental evidence of the chaotic regime in a salicylate biosensor 264 (1997) 662
Kück, S., see Hazenkamp, M.F. 265 (1997) 264
Kudelski, A., see Bukowska, J. 268 (1997) 481
Kukolich, S.G., see Sickafoose, S.M. 263 (1996) 191
Kukovitskii, E.F., L.A. Chernozatonskii, S.G. L'vov and N.N. Mel'nik, Carbon nanotubes of polyethylene 266 (1997) 323
Kulshrestha, S.K., see Majumder, C. 261 (1996) 515
Kumada, T., K. Komaguchi, Y. Aratono and T. Miyazaki, A remarkable temperature dependence of the rate constant for the tunneling reaction HD + D → H + D_2 in the low temperature region 2.6–6.5 K 261 (1996) 463
Kumada, T., see Komaguchi, K. 268 (1997) 493
Kumakura, M., see Yamazaki, T. 265 (1997) 137
Kumar, A., C.-C. Hsiao, W.-C. Hung and Y.-P. Lee, Effect of polarization on stimulated emission pumping spectroscopy of the $B^3\Pi_{0^+u}$–$X\,^1\Sigma_g^+$ system of jet-cooled Br_2 via two-colour resonant four-wave mixing 269 (1997) 22
Kumar, G.R., see Sevian, A. 263 (1996) 241
Kumaran, S.S., M.-C. Su and J.V. Michael, Thermal decomposition of iodobenzene using I-atom absorption 269 (1997) 99
Kumble, R., S. Palese, R.W. Visschers, P.L. Dutton and R.M. Hochstrasser, Ultrafast dynamics within the B820 subunit from the core (LH-1) antenna complex of *Rs. rubrum* 261 (1996) 396
Kummrow, A., see Lau, A. 263 (1996) 435
Kundu, T.K. and P.T. Manoharan, An electron paramagnetic resonance investigation of a macrobicyclic cage complex of Ag(II). Dynamic and static Jahn–Teller distortions 264 (1997) 338
Kunugi, Y., see Harima, Y. 267 (1997) 481
Küppers, J., see Kammler, Th. 267 (1997) 391
Kurawaki, J., Y. Sameshima and Y. Kusumoto, Conformation-dependent energy transfer for chlorophyll–copolypeptide complexes in an aqueous surfactant solution 266 (1997) 353
Kurokawa, S., see Teki, Y. 270 (1997) 573
Kusaba, M., see Suzuki, T. 263 (1996) 197
Kusumoto, Y., see Kurawaki, J. 266 (1997) 353
Kutzelnigg, W., see Cencek, W. 266 (1997) 383

Kwok, W.M. and D.L. Phillips, Gas and solution phase chloroiodomethane short-time photodissociation dynamics in the B-band absorption 270 (1997) 506
Kwok, W.M., D.L. Phillips, P.K.-Y. Yeung and V.W.-W. Yam, Vibrational reorganizational energies of the MLCT transition in $Pt(dppm)_2(PhC{\equiv}C)_2$ and the MMLCT transition in $[Pt_2(\mu\text{-dppm})_2(\mu\text{-PhC}{\equiv}C)(PhC{\equiv}C)_2]^+$ 262 (1996) 699
Kwok, W.M., W. Fuss and D.L. Phillips, Bond selective electronic excitation in $IC_2H_4C_2F_4I$ investigated by resonance Raman spectroscopy 261 (1996) 685

Labouriau, A. and W.L. Earl, Titanium solid-state NMR in anatase, brookite and rutile 270 (1997) 278
Lacey, J.A., see Henari, F.Z. 267 (1997) 229
Laganà, A., P. Spatola, G. Ochoa de Aspuru, G. Ferraro and O. Gervasi, Eigensolutions for one-dimensional cuts of bond order potentials 267 (1997) 403
Lahem, D., R. Flammang and M.T. Nguyen, Observation of thiohydroxy-hydroxy-carbene [HS–C–OH] when searching for thionformic acid [HC(=S)OH] in the gas phase 270 (1997) 93
Lai, R., see Mungan, C.E. 270 (1997) 309
Laible, P.D., see Chen, L.X. 270 (1997) 255
Lallemand, J.-Y., see Abergel, D. 262 (1996) 465
La Manna, G., see Ciofalo, M. 263 (1996) 73
Lambert, H.M., see Eng, R. 261 (1996) 651
Lambert, R.M., see Lomas, J.R. 263 (1996) 591
Lamberti, C., G. Spoto, D. Scarano, C. Pazé, M. Salvalaggio, S. Bordiga, A. Zecchina, G. Turnes Palomino and F. D'Acapito, Cu^I–Y and Cu^{II}–Y zeolites: a XANES, EXAFS and visible–NIR study 269 (1997) 500
Lankers, M., see Trunk, M. 264 (1997) 233
Lanzani, G., M. Nisoli, S. De Silvestri and F. Abbate, Exciton dynamics in α-sexithienyl films 264 (1997) 667
Larson, E.J., L.A. Friesen and C.K. Johnson, An ultrafast one-photon and two-photon transient absorption study of the solvent-dependent photophysics in all-trans retinal 265 (1997) 161
Larzillière, M., see Roney, A. 270 (1997) 59
Lascola, R. and J.C. Wright, Measurement of the second order molecular hyperpolarizability of C_{60}^- by nondegenerate four-wave mixing 269 (1997) 79
Latifzadeh-Masoudipour, L. and K. Balasubramanian, Electronic states and potential energy curves of PI_2 and PI_2^+ 267 (1997) 545
Latifzadeh-Masoudipour, L. and K. Balasubramanian, Electronic states and potential energy curves of SbF_2 and SbF_2^+ 262 (1996) 553
Lau, A., M. Pfeiffer and A. Kummrow, Subpicosecond two-dimensional Raman spectroscopy applying broadband nanosecond laser radiation 263 (1996) 435
Lau, A., see Werncke, W. 266 (1997) 99
Lau, A., see Pfeiffer, M. 268 (1997) 258
Lau, K.H., see Hildenbrand, D.L. 263 (1996) 145
Lauenstein, C., see Baumfalk, R. 269 (1997) 321
Laufer, G. and A.S. Lee, Water assisted multi-photon ionization of N_2 by KrF lasers 266 (1997) 584
Laurent, T., see Brownsword, R.A. 266 (1997) 259
Lavendy, H., see Robbe, J.M. 267 (1997) 91
Lavín, C., see Velasco, A.M. 264 (1997) 579
Lay, T.H. and J.W. Bozzelli, Enthalpies of formation of cyclic alkyl peroxides: dioxirane, 1,2-dioxetane, 1,2-dioxolane, and 1,2-dioxane 268 (1997) 175
Lazarou, Y.G., see Kambanis, K.G. 261 (1996) 457

Lazarou, Y.G., see Kambanis, K.G. 268 (1997) 498
Leal Ferreira, G.F., see Mergulhão, S. 269 (1997) 489
Lebedkin, S., see Gromov, A. 267 (1997) 460
Le Bras, G., see Bedjanian, Y. 266 (1997) 233
Le Coat, Y., see Hedhili, M.N. 268 (1997) 21
Le Doucen, R., see Khalil, B. 263 (1996) 811
Lee, A.S., see Laufer, G. 266 (1997) 584
Lee, E.S., see Kim, D.-C. 265 (1997) 573
Lee, H.M., see Batirev, I.G. 262 (1996) 247
Lee, J.Y., see Kim, K.S. 265 (1997) 497
Lee, K., H.S. Yoo and J.K. Ku, Ground state Fe atom formation efficiencies from two-photon dissociation of $Fe(CO)_5$ at 386.0, 368.0, 319.3 and 298.4 nm 262 (1996) 610
Lee, K.H., see Batirev, I.G. 262 (1996) 247
Lee, M.-H., C.-F. Cheng, V. Heine and J. Klinowski, Distribution of tetrahedral and octahedral Al sites in gamma alumina 265 (1997) 673
Lee, S., K. Arita and O. Kajimoto, Laser-induced fluorescence excitation spectrum of jet-cooled 4-(9-anthryl)aniline: observation of two weakly coupled electronic states 265 (1997) 579
Lee, S., Density functional study of polycarbon sulfides C_nS ($n = 2–9$) 268 (1997) 69
Lee, S., see Oishi, O. 269 (1997) 530
Lee, S.A. and A. Anderson, Deuterated methylene iodide at high pressures: a Raman study 262 (1996) 337
Lee, S.S., see Kong, M.J. 263 (1996) 1
Lee, T.-S., see York, D.M. 263 (1996) 297
Lee, T.G., Y.M. Rhee, M.S. Kim and S.C. Park, Energy partitioning during the exit channel motion for $CH_2OH^+ \rightarrow CHO^+ + H_2$ 264 (1997) 303
Lee, T.J., Ab initio characterization of $HBrO_2$ isomers: implications for stratospheric bromine chemistry 262 (1996) 559
Lee, W.R., see Batirev, I.G. 262 (1996) 247
Lee, Y.-P., see Kumar, A. 269 (1997) 22
Lee, Y.H., S.G. Kim and D. Tománek, Field-induced unraveling of carbon nanotubes 265 (1997) 667
Lee, Y.H., see Kim, S.G. 264 (1997) 345
Lefebvre-Brion, H., Biexponential decay of peak intensities in the zero electron kinetic energy pulsed field ionization of HCl 268 (1997) 107
Lefèvre, J.-P., see Fedorov, A. 267 (1997) 467
Le Garrec, J.L., V. Lepage, B.R. Rowe and E.E. Ferguson, The temperature dependence of the rate constant for $O^+ + NO \rightarrow NO^+ + O$ from 23 to 30000 K 270 (1997) 66
Legon, A.C., see Cooke, S.A. 262 (1996) 308
Legon, A.C., see Cooke, S.A. 266 (1997) 61
Legon, A.C., see Evans, C.M. 267 (1997) 281
Legon, A.C., see Cotti, G. 264 (1997) 513
Legrand, J.-C., see Diamy, A.-M. 269 (1997) 327
Leicknam, J.-.C., see Bratos, S. 261 (1996) 117
Leiro, J.A., see Batirev, I.G. 262 (1996) 247
Lemmetyinen, H., see Tkachenko, N.V. 261 (1996) 234
Lennon, D., see Kidd, R.T. 262 (1996) 142
Lenz, K., see Pfeiffer, M. 268 (1997) 258
Leone, S.R., see Williams, R.M. 261 (1996) 405
Leonhardt, M., see Gómez, U. 268 (1997) 1
Lepage, V., see Le Garrec, J.L. 270 (1997) 66

Lequeux, F., see Menon, S.V.G. 263 (1996) 727
Lesar, A., see Kokalj, A. 268 (1997) 43
Leszczynski, J., see Urban, J. 264 (1997) 441
Leupold, D., see Teuchner, K. 268 (1997) 157
Leutwyler, S., see Sabo, D. 261 (1996) 318
Leutwyler, S., see Wickleder, C. 264 (1997) 257
Lev-On, T., see Kandel, S.A. 265 (1997) 121
Levine, R.D., see Ben-Nun, M. 270 (1997) 319
Levis, R.J., see Velic, D. 269 (1997) 59
Levstein, P.R., see Pastawski, H.M. 261 (1996) 329
Levy, R.M., see Del Buono, G.S. 263 (1996) 521
Li, B.Z., see Allen, M.D. 270 (1997) 517
Li, F., Y. Lu, G. Xue and Q. Cao, The adsorption and bonding of ω-mercaptoalkanols on HNO_3 etched copper 264 (1997) 376
Li, H., D. Biglino, R. Erickson and A. Lund, The structure of a copper(II) complex with water in Cu-ZSM-5 at 4 K by ENDOR 266 (1997) 417
Li, H., see Chan, C.M.-T. 269 (1997) 49
Li, J., see Li, Y. 265 (1997) 361
Li, L., T. He, X. Wang, J. Zuo, C. Xu and F. Liu, Contribution of antisymmetric nonresonant vibrational Raman scattering to the ν_{16} and ν_{17} bands of tetrahydrofuran 262 (1996) 52
Li, L., T. He, X. Wang and F.-C. Liu, Laser-induced ESR shift from the contribution of the symmetric polarizability 268 (1997) 549
Li, L., see Antonova, S. 267 (1997) 158
Li, L., see Guo, L.P. 268 (1997) 26
Li, Q. and L. Luo, A study of the growth rates and growth habits of ice crystals in a solution of antifreeze (glyco)proteins 263 (1996) 651
Li, Q., see Han, W. 265 (1997) 374
Li, R.-J., see Arusi-Parpar, T. 268 (1997) 163
Li, S., R.J. Van Zee and W. Weltner Jr., Infrared observations of the B_3 and Al_3 molecules in inert-gas matrices at 4 K 262 (1996) 298
Li, S.Y., see Hrbek, J. 267 (1997) 65
Li, X., P. Pircher, D. Gruber and L. Windholz, The LiHg $X\,^2\Sigma^+ \rightarrow 2\,^2\Pi_{3/2}$ transition: excitation spectrum and rotational analysis of the $v'' = 0$–$v' = 1$ band 263 (1996) 463
Li, Y., Z. Mao, J. Xu, J. Yang, Z. Guo, D. Zhu, J. Li and B. Yin, Preparation of a novel stable nitroxide based on [60]fulleropyrrolidine and its magnetic properties 265 (1997) 361
Li, Y., E. Blaisten-Barojas and D.A. Papaconstantopoulos, Molecular dynamics study of neutral and multiply charged sodium clusters 268 (1997) 331
Li, Y., see Zhao, L. 263 (1996) 235
Li, Z., Ab initio study on the dissociation pathways of XSO_2 (X = Cl, F) radicals 269 (1997) 128
Li, Z.H., see Huang, H.H. 265 (1997) 508
Liang, J., see Bauer-Gogonea, S. 262 (1996) 663
Liang, W., see Han, W. 265 (1997) 374
Liao, M.-S., see Au, C.T. 267 (1997) 44
Lichanot, A., see Rérat, M. 263 (1996) 767
Lidzey, D.G., M.A. Pate, D.M. Whittaker, D.D.C. Bradley, M.S. Weaver, T.A. Fisher and M.S. Skolnick, Control of photoluminescence emission from a conjugated polymer using an optimised microcavity structure 263 (1996) 655
Liebermann, H.-P., see Wright, J.S. 266 (1997) 391

Liedl, K.R., see Remko, M. 263 (1996) 379
Lifshitz, C., see Matt, S. 264 (1997) 149
Limantara, L., I. Katheder, H. Scheer, W. Schäfer and Y. Koyama, The T_1 and S_1 Raman spectra of ^{15}N- and ^{2}H-enriched bacteriochlorophyll *a*: changes in bond order upon triplet and singlet excitation 262 (1996) 656
Lin, L., see Engeln, R. 269 (1997) 293
Lin, L.-R., Y.-B. Jiang, X. Du, X.-Z. Huang and G. Chen, A study of the properties of the 1 : 1 inclusion complex of β-cyclodextrin with cetyltrimethylammonium bromide 266 (1997) 358
Lin, L.-R., see Du, X.-Z. 268 (1997) 31
Lin, N., see Ding, J. 261 (1996) 92
Lin, S.H., see Brezina, R. 262 (1996) 437
Lin, S.H., see Der Chao, S. 265 (1997) 445
Lindan, P.J.D., N.M. Harrison, J.M. Holender and M.J. Gillan, First-principles molecular dynamics simulation of water dissociation on TiO_2 (110) 261 (1996) 246
Lindgren, B., see Doverstål, M. 270 (1997) 273
Lindinger, M., see Walther, C. 262 (1996) 668
Lingott, R., see Wright, J.S. 266 (1997) 391
Liou, H.T., K.L. Huang and M.C. Chen, The rotationally resolved spectra and pre-dissociation of CS_2 of 210 nm band initiated from highly vibrationally excited levels 266 (1997) 591
Lipiński, J. and L. Komorowski, The solvent effect on the electronegativity and hardness of bonded atoms 262 (1996) 449
Lipsky, S., see Saik, V.O. 264 (1997) 649
Lipson, S.J., see Bieniek, R.J. 263 (1996) 276
Liszi, J., see Kristóf, T. 261 (1996) 620
Liu, F., see Li, L. 262 (1996) 52
Liu, F.-C., see Li, L. 268 (1997) 549
Liu, R., see Huang, Y. 268 (1997) 365
Liu, S., see López-Boada, R. 270 (1997) 443
Liu, S., see Wang, Y.A. 267 (1997) 14
Liu, W.-K., see Brezina, R. 262 (1996) 437
Liu, Z.F., see Zhu, T. 265 (1997) 334
Lizzit, S., see Comelli, G. 261 (1996) 253
Lo, C.F., Squeezed states of molecular vibrations 267 (1997) 411
Lo, K.K.-W., see Wang, C.-R. 262 (1996) 91
Lobanov, A.N., see Argyrakis, P. 268 (1997) 372
Lomas, J.R., C.J. Baddeley, M.S. Tikhov and R.M. Lambert, On the orientation of benzene adsorbed on Cu{110} 263 (1996) 591
Longo, S., Chemical instabilities in the XeCl laser discharge: a stochastic approach 268 (1997) 306
Longo, S., see Capitelli, M. 263 (1996) 635
López-Boada, R., V. Karasiev and S. Liu, Padé approximation for the polynomial representation of the correlation energy density functional 270 (1997) 443
Lopez, M. and D.J.S. Birch, Characterisation of the dimer formed by hydrolysis of uranyl in aqueous solution and its role in the biexponential luminescence decay 268 (1997) 125
Loppnow, G.R., see Mitambo, M.M. 261 (1996) 691
Lorents, D.C., see Shen, H. 264 (1997) 508
Lorentzen, J.D., S. Guha, J. Menéndez, P. Giannozzi and S. Baroni, Raman cross section for the pentagonal-pinch mode in buckminsterfullerene C_{60} 270 (1997) 129

Lorenz, K.T., K.A. Cowen, P.E. Fleming, M.G. Mathews, M.F. Herman and B. Koplitz, Toward understanding the role of Stark effects when probing the nuclear hyperfine states of atomic hydrogen 261 (1996) 145
Lou, N., see Ding, G. 265 (1997) 392
Lou, N.-Q., see Zhan, J.-P. 264 (1997) 687
Louis-Joseph, A., see Abergel, D. 262 (1996) 465
L.Richardson, S., J.S. Francisco, A.M. Mebel and K. Morokuma, Can chlorine anion catalyze the reaction of HOCl with HCl? 270 (1997) 395
Lu, X., see Fang, J. 270 (1997) 145
Lu, Y., see Li, F. 264 (1997) 376
Lu, Z., see Fang, J. 270 (1997) 145
Lubitz, W., see Zweygart, W. 261 (1996) 272
Lucas, J.M., see Romero, T. 261 (1996) 583
Lucchese, R.R., see Han, J. 265 (1997) 209
Luchinat, C., see Bertini, I. 265 (1997) 677
Lüchow, A., see Mella, M. 265 (1997) 467
Lüder, C., D. Prekas, A. Vourliotaki and M. Velegrakis, Photodissociation spectrum of Sr^+Ne 267 (1997) 149
Luna, A., B. Amekraz and J. Tortajada, A theoretical study on the complexation of sp, sp^2 and sp^3 nitrogen-containing species by Cu^+ 266 (1997) 31
Lund, A., see Komaguchi, K. 265 (1997) 217
Lund, A., see Li, H. 266 (1997) 417
Lundell, J., Ab initio study of the HCOOH–Ar van der Waals complex 266 (1997) 1
Luo, L., see Li, Q. 263 (1996) 651
Luo, R.-S. and X.-A. Mao, Observation of the exchange of small molecules between phases in a SDS micellar system 270 (1997) 77
Luque, F.J., see Orozco, M. 265 (1997) 473
Lüthi, H.P., see Klopper, W. 262 (1996) 546
Lützenkirchen, K., see Walther, C. 262 (1996) 668
L'vov, S.G., see Kukovitskii, E.F. 266 (1997) 323
Lyapustina, S.A., see Tsukuda, T. 269 (1997) 17
Lyubovitsky, J., see Kong, M.J. 263 (1996) 1
Lyyra, A.M., see Antonova, S. 267 (1997) 158

Ma, Z.-Q., see Xie, M. 262 (1996) 1
Maas, D.J., D.I. Duncan, A.F.G. van der Meer, W.J. van der Zande and L.D. Noordam, Vibrational ladder climbing in NO by ultrashort infrared laser pulses 270 (1997) 45
Maas, F.E., see Yamazaki, T. 265 (1997) 137
Maccaferri, G., see Caminati, W. 265 (1997) 561
Maccaferri, G., see Melandri, S. 261 (1996) 267
Machado, J.C., see Porto, A.O. 266 (1997) 329
Mack, H.-G., see Gobbato, K.I. 266 (1997) 527
Maclagan, R.G.A.R. and G.E. Scuseria, An ab initio study of VC: a comparison of different levels of theory including density functional methods 262 (1996) 87
Macsári, I., V. Izvekov and A. Kovács, Scaled quantum mechanical study of 2,6-di-fluorophenol: a fluorine-containing weak hydrogen-bonded system 269 (1997) 393
Madej, C., see Zhang, L. 268 (1997) 408

Mádi, Z.L., B. Brutscher, T. Schulte-Herbrüggen, R. Brüschweiler and R.R. Ernst, Time-resolved observation of spin waves in a linear chain of nuclear spins 268 (1997) 300
Maeda, K., Y. Araki, Y. Kamata, K. Enjo, H. Murai and T. Azumi, The time-resolved absorption-detected magnetic resonance spectrum of the polymethylene linked biradical: effect of the exchange integral 262 (1996) 110
Maeda, K., see Ali, S.S. 267 (1997) 520
Maeda, K., see Murai, H. 264 (1997) 619
Maes, G., see Smets, J. 262 (1996) 789
Maeyama, T., T. Tsumura, A. Fujii and N. Mikami, Photodetachment of small water cluster anions in the near-infrared through the visible region 264 (1997) 292
Magalhães, W.F., see Porto, A.O. 266 (1997) 329
Magnier, S., M. Persico and N. Rahman, Bound–bound and bound–free $X^2\Sigma_g^+ \rightarrow A^2\Pi_u$ transitions in Na_2^+ relevant for experiments in above threshold dissociation 262 (1996) 747
Mahapatra, U.S., see Mitra, A. 261 (1996) 363
Maier, J.P., see Kotterer, M. 266 (1997) 342
Maier, J.P., see Meuwly, M. 270 (1997) 252
Maier, J.P., see Nizkorodov, S.A. 265 (1997) 303
Maierle, C.S. and R.A. Harris, Spin one-half optical activity 267 (1997) 199
Majumdar, D. and K. Balasubramanian, A theoretical study of the curves for Ta + CO interaction 262 (1996) 263
Majumder, C., G.P. Das, S.K. Kulshrestha, V. Shah and D.G. Kanhere, Ground state geometries and energetics of Al_nLi ($n = 1, 13$) clusters using ab initio density-based molecular dynamics 261 (1996) 515
Makarov, E.F., see Aleinikov, N.N. 267 (1997) 155
Makarov, V.I., Yu.N. Molin, S.A. Kochubei and V.N. Ishchenko, Microwave field effect on the fluorescence of $(COF)_2$ excited to the 0_0^0 band of the $\tilde{A}^1A_u$ state 266 (1997) 303
Makarshin, L.L., D.V. Andreev and V.N. Parmon, 'Levitation' of paramagnetic oxygen molecules over the surface of high temperature superconductors 266 (1997) 173
Maki, S., see Waga, M. 265 (1997) 277
Malagoli, M., see Cross, G.H. 268 (1997) 36
Maldivi, P., see Adamo, C. 268 (1997) 61
Malisch, W., see Markert, T. 270 (1997) 222
Malkin, V.G., O.L. Malkina and D.R. Salahub, Spin–orbit correction to NMR shielding constants from density functional theory 261 (1996) 335
Malkin, V.G., see Kaupp, M. 265 (1997) 55
Malkina, O.L., see Kaupp, M. 265 (1997) 55
Malkina, O.L., see Malkin, V.G. 261 (1996) 335
Málková, Z., see Rodová, M. 268 (1997) 455
Malmqvist, P.-Å., see Christiansen, O. 261 (1996) 369
Malrieu, J.-P., see Reguero, M. 265 (1997) 621
Malrieu, J.P., see García, V.M. 261 (1996) 98
Manciu, M., see Mishori, B. 264 (1997) 163
Mandal, A.B., see Baskar, G. 266 (1997) 443
Manero, F., see García, G. 264 (1997) 589
Maniwa, Y., see Qin, L.-C. 268 (1997) 101
Manners, I., see Masoumi, Z. 261 (1996) 551
Manohar, C., see Menon, S.V.G. 263 (1996) 727
Manoharan, P.T., see Kundu, T.K. 264 (1997) 338

Manoj, N. and K.R. Gopidas, Structure–photophysics correlation in a series of 2,6-dimethyl-4-arylpyrylium derivatives 267 (1997) 567
Mansfield, M.W.D., see Ruth, A.A. 264 (1997) 605
Mao, H.-F., see Tian, H.-J. 263 (1996) 471
Mao, X.-A., see Luo, R.-S. 270 (1997) 77
Mao, Z., see Li, Y. 265 (1997) 361
Marchettini, N., see Rustici, M. 263 (1996) 429
Marian, C.M., see Bündgen, P. 261 (1996) 625
Marijnissen, A. and J.J. ter Meulen, Determination of the adiabatic ionization potentials of Si_2 and SiCl by photoionization efficiency spectroscopy 263 (1996) 803
Maris, A., see Melandri, S. 261 (1996) 267
Märk, T.D., see Matejcik, S. 261 (1996) 437
Märk, T.D., see Senn, G. 266 (1997) 276
Märk, T.D., see Matt, S. 264 (1997) 149
Märk, T.D., see Matejcik, S. 267 (1997) 329
Märk, T.D., see Wörgötter, R. 270 (1997) 333
Markert, T., W. Malisch and V. Engel, Vibrational dynamics and energy flow in a multi-mode organometallic compound 270 (1997) 222
Marqueton, Y., see Even, J. 267 (1997) 585
Marsden, C., see Smart, B. 261 (1996) 51
Marshall, P., A. Misra and R.J. Berry, Computational studies of the reactions of CH_3I with H and OH 265 (1997) 48
Marshall, P., see Berry, R.J. 269 (1997) 107
Martin, I., see Velasco, A.M. 264 (1997) 579
Martin, J.C., see Ambrose, W.P. 269 (1997) 365
Martin, J.M.L., The vibrational spectra of corannulene and coronene. A density functional study 262 (1996) 97
Martin, M. and M. Castillejo, Vibrational and rotational dependence of the removal of $CD(A\,^2\Delta, B\,^2\Sigma^-$ and $C\,^2\Sigma^+)$ by H_2 266 (1997) 111
Martín, M., see Castillejo, M. 268 (1997) 465
Martin, P.A., see Fehér, M. 261 (1996) 23
Martin, S.E., see Ball, S.M. 264 (1997) 531
Martinez, R., see Alvarez-Ramirez, J. 266 (1997) 375
Martínez, T.J., see Ben-Nun, M. 262 (1996) 405
Martínez, T.J., see Ben-Nun, M. 270 (1997) 319
Martrenchard-Barra, S., see Dedonder-Lardeux, C. 264 (1997) 596
Marx, N.J., see Müller, R. 262 (1996) 716
Maslen, P.E., J. Faeder and R. Parson, Ab initio calculations of the ground and excited states of I_2^- and ICl^- 263 (1996) 63
Maslen, P.E., see Faeder, J. 270 (1997) 196
Masoumi, Z., V. Stoeva, A. Yekta, Z. Pang, I. Manners and M.A. Winnik, Luminescence quenching method for probing the diffusivity of molecular oxygen in highly permeable media 261 (1996) 551
Masters, A.J., see Akhmatskaya, E.V. 267 (1997) 105
Mataga, N., see Chosrowjan, H. 270 (1997) 267
Mataga, N., see Kotani, S. 269 (1997) 274
Matejcik, S., P. Cicman, A. Kiendler, G. Senn, E. Illenberger and T.D. Märk, Electron transfer processes in binary van der Waals clusters via the $N_2^-(^2\Pi_g)$ resonance 267 (1997) 329

Matejcik, S., P. Cicman, A. Kiendler, J.D. Skalny, E. Illenberger, A. Stamatovic and T.D. Märk, Low-energy electron attachment to mixed ozone/oxygen clusters 261 (1996) 437
Materny, A., see Schmitt, M. 270 (1997) 9
Mathews, M.G., see Lorenz, K.T. 261 (1996) 145
Mathies, R.A., see Kauffmann, E. 266 (1997) 554
Mathur, D., see Vijayalakshmi, K. 270 (1997) 37
Mathur, D., see Shen, H. 264 (1997) 508
Matsubara, M., see Ishiguro, M. 263 (1996) 629
Matsuda, H., see Kobayashi, T. 267 (1997) 472
Matsui, A.H., see Takeshima, M. 266 (1997) 135
Matsuo, S. and T. Tahara, Phase-stabilized optical heterodyne detection of impulsive stimulated Raman scattering 264 (1997) 636
Matsushima, T., see Yamanaka, T. 264 (1997) 180
Matsuyama, A., see Murai, H. 264 (1997) 619
Matsuzaki, Y., M. Nakano, K. Yamaguchi, K. Tanaka and T. Yamabe, Third-order optical nonlinearity in new π-conjugated polymers: polydiethynylsilane and polysilole 263 (1996) 119
Matt, S., O. Echt, R. Wörgötter, V. Grill, P. Scheier, C. Lifshitz and T.D. Märk, Appearance and ionization energies of multiply-charged C_{70} parent ions produced by electron impact ionization 264 (1997) 149
Mayer, I., G. Räther and S. Suhai, The chemical Hamiltonian approach for infinite chains 270 (1997) 211
Mayer, P.M. and T. Baer, The heat of formation of $ClSO^+$ 261 (1996) 155
Mayne, H.R., see Niesse, J.A. 261 (1996) 576
McAvoy, T., see McIlroy, D.N. 264 (1997) 168
McCaffery, A.J., see Wilson, R.J. 261 (1996) 195
McCarthy, M.C., M.J. Travers, P. Kalmus, C.A. Gottlieb and P. Thaddeus, Microwave spectroscopy of the carbon chain radical $C_{11}H$ 264 (1997) 252
McCourt, F.R.W., see Wang, F. 269 (1997) 138
McDowell, C.A., see Ding, S. 270 (1997) 81
McDowell, C.A., see Ding, S. 268 (1997) 194
McDowell, S.A.C., Interatomic potentials for $ArLi^+$ obtained by SCF, MP2 and density functional theory 266 (1997) 38
McEwan, M.J., see Scott, G.B.I. 269 (1997) 88
McGrother, S.C., see Gil-Villegas, A. 269 (1997) 441
McHale, J.L., see Britt, B.M. 270 (1997) 551
McIlroy, D.N., C. Waldfried, T. McAvoy, J. Choi, P.A. Dowben and D. Heskett, The nonmetal to metal transition with alkali doping of films of molecular icosahedra 264 (1997) 168
McIntosh, A.L., see Han, J. 265 (1997) 209
McIntosh, A.L., see Han, J. 264 (1997) 411
McOrist, G., see Gadd, G.E. 270 (1997) 108
McQuillan, A.J., see Duffy, N.W. 266 (1997) 451
Mebel, A.M., see L.Richardson, S. 270 (1997) 395
Medhurst, L.J., J. Fleming and H.H. Nelson, Reaction rate constants of $OH + CHF_3 \rightarrow$ products and $O(^3P) + CHF_3 \rightarrow OH + CF_3$ at 500–750 K 266 (1997) 607
Meech, S.R., see Kidd, R.T. 262 (1996) 142
Meerts, W.L., see Drabbels, M. 267 (1997) 127
Meier, B.H., see Verhoeven, A. 266 (1997) 465
Meijer, B., see Hendrickx, E. 270 (1997) 241
Meijer, G., see Berden, G. 265 (1997) 204

Meijer, G., see Engeln, R. 262 (1996) 105
Meijer, G., see Jongma, R.T. 270 (1997) 304
Meijer, G., see Warntjes, J.B.M. 261 (1996) 495
Meijer, G., see Engeln, R. 269 (1997) 293
Meijerink, A., see van Dijken, A. 269 (1997) 494
Meissner, L., A posteriori corrections to the configuration interaction method with singles and doubles 263 (1996) 351
Meixner, A.J., see Bopp, M.A. 263 (1996) 721
Melandri, S., G. Maccaferri, A. Maris, A. Millemaggi, W. Caminati and P.G. Favero, Observation of the rotational spectra of van der Waals complexes by free jet absorption millimeter wave spectroscopy: pyridine–argon 261 (1996) 267
Melandri, S., see Caminati, W. 268 (1997) 393
Meléndez, F.J., M.L. Senent and Y.G. Smeyers, The effects of the C=O wagging coordinate relaxation on the far-infrared torsional spectrum of acetone 265 (1997) 649
Melicherčík, M., see Olexová, A. 268 (1997) 505
Mella, M., A. Lüchow and J.B. Anderson, An improved transition matrix for variational quantum Monte Carlo 265 (1997) 467
Mello, C., see Kubota, L.T. 264 (1997) 662
Mel'nik, N.N., see Kukovitskii, E.F. 266 (1997) 323
Mendes, L.G., see de Souza, I.C.L. 264 (1996) 584
Menéndez, J., see Lorentzen, J.D. 270 (1997) 129
Meng, Q.B., see Wu, Z.J. 267 (1997) 271
Menon, S.V.G., C. Manohar and F. Lequeux, Vesicle to micelle transitions induced by Coulomb correlations in two dimensions 263 (1996) 727
Menzel, D., see Narloch, B. 270 (1997) 163
Merckens, H.-P., see Hilger, R. 262 (1996) 400
Merelas, I., see Fernández, J.A. 267 (1997) 301
Mergulhão, S., R.M. Faria, G.F. Leal Ferreira and J. Sworakowski, Transport of holes in uniformly and non-uniformly protonated poly(*o*-methoxyaniline) 269 (1997) 489
Merkt, F., see Palm, H. 270 (1997) 1
Mertz, E.L., On the dependence of the electron band maximum on the solvent reorganization energy 262 (1996) 27
Merzel, F., Direct orbital-free calculations using DFT and one-electron Green's functions: applications to atoms 263 (1996) 507
Metcalf, D.H., see Dai, S. 262 (1996) 315
Meunier, H., P. Pagsberg and A. Sillesen, Kinetics and branching ratios of the reactions $NH_2 + NO_2 \rightarrow N_2O + H_2O$ and $NH_2 + NO_2 \rightarrow H_2NO + NO$ studied by pulse radiolysis combined with time-resolved infrared diode laser spectroscopy 261 (1996) 277
Meuwly, M., S.A. Nizkorodov, E.J. Bieske, J.P. Maier and O. Dopfer, Reply to the Comment on ''The ν_3 infrared spectrum of the He–NH_4^+ complex'' 270 (1997) 252
Meyer, H., Rotational contour analysis of the (n, 3s) Rydberg transition in acetaldehyde 262 (1996) 603
Meyer, R., see Caminati, W. 268 (1997) 393
Meyer, Y.H., P. Plaza and K. Müllen, Ultrafast spectroscopy of soluble terrylene and quaterrylene 264 (1997) 643
Miaskiewicz, K. and D.A. Smith, Computational density functional theory vibrational spectra of cubane 270 (1997) 376
Michael, J.V., see Kumaran, S.S. 269 (1997) 99
Michel, R.H., see Cummins, T.R. 261 (1996) 228

Michl, J., see Imhof, R. 270 (1997) 500
Middelhoek, E.R., H. Zhang, J.W. Verhoeven and M. Glasbeek, Subpicosecond time-dependent Stokes shift studies of the donor–acceptor compound PIDMP in ethereal solution 267 (1997) 525
Mikami, N., see Maeyama, T. 264 (1997) 292
Mikhailov, A. and G. Ertl, Reply to Comment on ''Pattern formation by adsorbates with attractive lateral interactions'' 267 (1997) 400
Mikhailov, M.A., see Osad'ko, I.S. 270 (1997) 183
Miki, S., see Nakayama, T. 266 (1997) 601
Milani, P., see Biasioli, F. 270 (1997) 115
Milce, A.P., see Payne, M.A. 265 (1997) 244
Mile, B., P.D. Sillman and A.R. Yacob, The first ENDOR spectrum of naked metal clusters: $^{7}Li_3$, $^{6}Li\,^{7}Li_2$ and $^{7}Li_3(H_2O)_x$ in an adamantane matrix 263 (1996) 710
Milgrom, L.R., see Henari, F.Z. 267 (1997) 229
Millemaggi, A., see Melandri, S. 261 (1996) 267
Miller, S.M. and T. Carrington Jr., Calculation of reaction probabilities using wavepackets 267 (1997) 417
Miller, T.A., see Tserepi, A.D. 265 (1997) 297
Miller, W.H., see Poirier, B. 265 (1997) 77
Miller, W.H., see Spath, B.W. 262 (1996) 486
Minamitsu, A., see Hiraoka, K. 267 (1997) 580
Mingo, N. and Z. Knor, Trigonal images of transition metal atoms adsorbed on transition metal FCC (111) surfaces and their availability for scanning tunneling microscopy 263 (1996) 8
Minyaev, R.M., Double proton transfers in complexes of formic acid with CH_4, NH_3, H_2O, HF and H_2 262 (1996) 194
Miranda, P.B., V. Pflumio, H. Saijo and Y.R. Shen, Conformation of surfactant monolayers at solid/liquid interfaces 264 (1997) 387
Misawa, K., see Qiu, F. 266 (1997) 153
Mischler, B., see Radi, P.P. 265 (1997) 271
Mishori, B., Y. Shapira, A. Belu-Marian, M. Manciu and A. Devenyi, Studies of C_{60} thin films using surface photovoltage spectroscopy 264 (1997) 163
Mishra, S.P., D. Tiwary and M.C.R. Symons, Modes of electron loss from triphenyl phosphonium bromide: an unusual structural switch 263 (1996) 476
Misochko, E.Ya., see Goldschleger, A.U. 267 (1997) 288
Misra, A., see Marshall, P. 265 (1997) 48
Mitambo, M.M. and G.R. Loppnow, Raman spectroscopy: a structural probe of solute–solvent interactions in ethyl 4-(dimethylamino)benzoate 261 (1996) 691
Mitchell, D., see Seifert, G. 268 (1997) 352
Mitra, A., D. Sinha and U.S. Mahapatra, Open-shell coupled-cluster theory for a general incomplete model space using eigenvalue-independent partitioning 261 (1996) 363
Mitrović, M.M., Growth rate dispersion of small KDP crystals 265 (1997) 315
Mitsui, M., K. Takeda, Y. Kobori, A. Kawai and K. Obi, The first observation of CIDEP generated through the interaction between an excited singlet oxygen molecule and a free radical 262 (1996) 125
Mittal, J.P., see Ghosh, H.N. 265 (1997) 365
Mittal, J.P., see Mohan, H. 263 (1996) 263
Mittal, J.P., see Palit, D.K. 269 (1997) 286
Miura, Y., see Teki, Y. 270 (1997) 573

Miyasaka, H., T. Nobuto, A. Itaya, N. Tamai and M. Irie, Picosecond laser photolysis studies on a photochromic dithienylethene in solution and in crystalline phases 269 (1997) 281
Miyasaka, H., see Kotani, S. 269 (1997) 274
Miyatake, M., see Harima, Y. 262 (1996) 274
Miyawaki, J., see Nakanaga, T. 261 (1996) 414
Miyazaki, T., T. Uda, I. Štich and K. Terakura, Theoretical study of the structural evolution of small hydrogenated silicon clusters: Si_6H_x 261 (1996) 346
Miyazaki, T., see Kumada, T. 261 (1996) 463
Miyazaki, T., see Komaguchi, K. 268 (1997) 493
Miyoshi, E., see Noro, T. 261 (1996) 75
Mizutani, Y., see Kruglik, S.G. 266 (1997) 283
Mizutani, Y., see Zhao, X. 262 (1996) 643
Mó, O., see González, L. 263 (1996) 407
Mo, Y., Ch. Ottinger and T. Winkler, Molecular beam experiments clarifying conflicting reports on magnetic field effects in NO(B) afterglows 266 (1997) 267
Moazzen-Ahmadi, N., D.W.D. Sandilands and R.T. Boeré, Infrared diode laser spectroscopy of the ν_1 fundamental and the $\nu_1 + \nu_2 - \nu_2$ sequence bands of the CCO radical 265 (1997) 563
Möckel, H.J., see Pietzak, B. 265 (1997) 200
Mohan, H. and J.P. Mittal, Hydroxyl radical induced reactions with 1-bromo-2-fluorobenzene in aqueous solutions: formation of radical cations 263 (1996) 263
Moine, B., see Zhang, L. 268 (1997) 408
Mok, C.Y., see Huang, H.H. 265 (1997) 508
Moler, E.J., S.A. Kellar, W.R.A. Huff, Z. Hussain, Y. Zheng, E.A. Hudson, Y. Chen and D.A. Shirley, Adsorption site and structure determination of $c(2 \times 2)$ $N_2/Ni(100)$ using angle-resolved photoemission extended fine structure 264 (1997) 502
Molin, Yu.N., see Makarov, V.I. 266 (1997) 303
Molski, A., N. Boens and M. Ameloot, Transient effects can change identifiability criteria for complex excited-state processes 266 (1997) 139
Monshouwer, R., see Baltuška, A. 270 (1997) 263
Monshouwer, R., see Peterman, E.J.G. 264 (1997) 279
Moore, M.A., see Deng, L. 270 (1997) 299
Morais, J., see Chambers, S.A. 267 (1997) 51
Moreau, G., see Khalil, B. 263 (1996) 811
Morelli, J. and S. Hammes-Schiffer, Surface hopping and fully quantum dynamical wavepacket propagation on multiple coupled adiabatic potential surfaces for proton transfer reactions 269 (1997) 161
Morgan, P.L., see Gadd, G.E. 270 (1997) 108
Mori, W., see Kawakami, T. 261 (1996) 129
Moricca, S., see Gadd, G.E. 261 (1996) 221
Moricca, S., see Gadd, G.E. 270 (1997) 108
Morimoto, H., see Ueda, K. 261 (1996) 295
Morita, N., see Yamazaki, T. 265 (1997) 137
Morokuma, K., see Cui, Q. 263 (1996) 46
Morokuma, K., see Cui, Q. 263 (1996) 54
Morokuma, K., see Froese, R.D.J. 263 (1996) 393
Morokuma, K., see L.Richardson, S. 270 (1997) 395
Morrison, I.D., see Berry, A.J. 266 (1997) 195
Morse, M.D., see Brugh, D.J. 267 (1997) 370

Moszynski, R., F. de Weerd, G.C. Groenenboom and A. van der Avoird, He–HF scattering cross sections from an ab initio SAPT potential: confrontation with experiment 263 (1996) 107
Mota, F., see Novoa, J.J. 266 (1997) 23
Moulin, V., A. Schriver, L. Schriver-Mazzuoli and P. Chaquin, Infrared spectrum of 2,2,2-trichloroethanol isolated in gas matrices. Ab initio optimization of conformers and potential energy calculations 263 (1996) 423
Mühlpfordt, A., U. Even and N.P. Ernsting, Zero-kinetic-energy photoelectron spectroscopy and excited-state intramolecular proton transfer in a 'double' benzoxazole 263 (1996) 178
Mukamel, S., see Khidekel, V. 263 (1996) 350
Müllen, K., see Meyer, Y.H. 264 (1997) 643
Muller, J.F., see Hachimi, A. 268 (1997) 485
Müller, R., C. Zander, M. Sauer, M. Deimel, D.-S. Ko, S. Siebert, J. Arden-Jacob, G. Deltau, N.J. Marx, K.H. Drexhage and J. Wolfrum, Time-resolved identification of single molecules in solution with a pulsed semiconductor diode laser 262 (1996) 716
Müller, R., see Ko, D.-S. 269 (1997) 54
Müller, T. and P.H. Vaccaro, The application of pulsed slit-jet expansion sources in sub-Doppler degenerate four-wave mixing spectroscopy 266 (1997) 575
Müller, T., see Wasserman, T.A.W. 262 (1996) 329
Mullins, C.B., see Seets, D.C. 266 (1997) 431
Mulloni, V., D. Pedron and R. Bozio, Effects of the mixing of charge transfer and molecular excitations on the resonance Raman properties of symmetric radical dimers 263 (1996) 331
Munakata, M., see Ueda, K. 261 (1996) 295
Mungan, C.E., R. Lai and A.J. Sievers, Novel temperature dependence of the vibrational relaxation of SH^- in a two-state hopping system 270 (1997) 309
Munn, N.S. and D.C. Clary, Subsurface effects in the dissociation of H_2 on Pd(111) 266 (1997) 437
Muñoz-Crego, C. and J. Santamaría, The intermolecular relaxation of the NH stretching vibration of pyrrole in the liquid phase: a two-mode dynamical study 261 (1996) 569
Münster, A.F., see Stössel, R. 263 (1996) 789
Mura, M.E., P.J. Knowles and C.A. Reynolds, Potential energy surfaces from Kohn–Sham potentials 262 (1996) 533
Murai, H., A. Matsuyama, T. Ishida, Y. Iwasaki, K. Maeda and T. Azumi, Controlling of radical–ion pair reactions by microwave radiation: photoconductivity-detected magnetic resonance 264 (1997) 619
Murai, H., see Ali, S.S. 267 (1997) 520
Murai, H., see Kitahama, Y. 261 (1996) 160
Murai, H., see Maeda, K. 262 (1996) 110
Muravyov, A.A., see Butkovskaya, N.I. 266 (1997) 223
Mutzenhardt, P., see Canet, D. 264 (1996) 477
Myshlyavtsev, A.V., see Resnyanskii, E.D. 264 (1997) 174

Naaman, R., see Haran, A. 268 (1997) 475
Nachtigallová, D., M. Roeselová and R. Zahradník, Ab initio studies of the oxidation of methane with oxo-metal cations 270 (1997) 357
Nagahara, T., see Nakayama, T. 266 (1997) 601
Nagano, Y. and T. Nakamura, C_{60}–CCl_4 solvate: an AB_{13} type binary crystal 265 (1997) 358
Nagaoka, M., see Komatsuzaki, T. 265 (1997) 91
Nagase, S., see Kobayashi, K. 261 (1996) 502
Nagase, S., see Kobayashi, K. 262 (1996) 227

Nagase, Y., see Abe, J. 261 (1996) 18
Nagata, T., see Tsukuda, T. 268 (1997) 429
Nagi, G.K., see Coombes, D.S. 265 (1997) 532
Nagirnyi, V., M. Nikl, G.P. Pazzi and S. Zazubovich, Luminescence of a thallium-perturbed on-centre self-trapped exciton in CsCl:Tl crystal 268 (1997) 280
Nagpal, R., see Jiao, C.Q. 265 (1997) 239
Nagpal, R., see Jiao, C.Q. 269 (1997) 117
Naitoh, Y., see Saitow, K. 262 (1996) 621
Naitoh, Y., see Inokuchi, Y. 269 (1997) 298
Nakai, H., see Hidaka, M. 264 (1997) 371
Nakajima, A., see Judai, K. 270 (1997) 23
Nakajima, A., see Negishi, Y. 269 (1997) 199
Nakajima, S., see Kotani, S. 269 (1997) 274
Nakajima, T., see Kaneko, H. 261 (1996) 1
Nakamura, T., see Nagano, Y. 265 (1997) 358
Nakanaga, T., F. Ito, J. Miyawaki, K. Sugawara and H. Takeo, Observation of the infrared spectra of the NH_2-stretching vibration modes of aniline–Ar_n ($n = 1, 2$) clusters in a supersonic jet using REMPI 261 (1996) 414
Nakanaga, T., K. Sugawara, K. Kawamata and F. Ito, Infrared depletion spectroscopy of aniline–NH_3 and aniline–NH_3^+ clusters in a supersonic jet 267 (1997) 491
Nakanishi, H., see Kobayashi, T. 267 (1997) 472
Nakano, H., see Kawashima, Y. 267 (1997) 82
Nakano, M., S. Kiribayashi, S. Yamada, I. Shigemoto and K. Yamaguchi, Theoretical study of the second hyperpolarizabilities of three charged states of pentalene. A consideration of the structure–property correlation for the sensitive second hyperpolarizability 262 (1996) 66
Nakano, M., see Matsuzaki, Y. 263 (1996) 119
Nakano, M., see Yamada, S. 267 (1997) 438
Nakano, M., see Yamada, S. 267 (1997) 445
Nakashima, K., see Tokeshi, M. 263 (1996) 783
Nakashima, N., see Chosrowjan, H. 270 (1997) 267
Nakashima, N., see Suzuki, T. 263 (1996) 197
Nakashima, S., M. Norimoto, H. Harima, Y. Hamanaka, L.S. Grigoryan and M. Tokumoto, Raman scattering of iodine intercalated C_{60} crystals 268 (1997) 359
Nakatsuji, H., see Hada, M. 261 (1996) 7
Nakatsuji, H., see Kaneko, H. 261 (1996) 1
Nakatsuji, H., see Hidaka, M. 264 (1997) 371
Nakayama, K., see Kawashima, Y. 267 (1997) 82
Nakayama, T., T. Nagahara, S. Miki and K. Hamanoue, Excited-state dynamics of naphthoylnaphthvalene: valence isomerization of the lowest excited singlet state and intermolecular hydrogen-atom abstraction of the lowest excited triplet state 266 (1997) 601
Nakayama, T., see Hamanoue, K. 267 (1997) 165
Namdas, E.B., see Deshpande, A.V. 263 (1996) 449
Napartovich, A.P., see Dyatko, N.A. 263 (1996) 305
Narloch, B. and D. Menzel, Structural evidence for chemical contributions in the bonding of the heavy rare gases on a close-packed transition metal surface: Xe and Kr on Ru(001) 270 (1997) 163
Nath, B., see Biswas, R. 263 (1996) 495

Nath, B., see Biswas, R. 269 (1997) 186
Naulin, C., I.M. Hedgecock and M. Costes, The dissociation energy of TiO determined from a crossed-beam study of the Ti + NO → TiO + N reaction 266 (1997) 335
Neelakandan, M., D. Pant and E.L. Quitevis, Reorientational and intermolecular dynamics in binary liquid mixtures of hexafluorobenzene and benzene: femtosecond optical Kerr effect measurements 265 (1997) 283
Negishi, Y., H. Kawamata, T. Hayase, M. Gomei, R. Kishi, F. Hayakawa, A. Nakajima and K. Kaya, Photoelectron spectroscopy of germanium–fluorine binary cluster anions: the HOMO–LUMO gap estimation of Ge_n clusters 269 (1997) 199
Neher, D., see Gelinck, G.H. 265 (1997) 320
Nelson, H.H., see Medhurst, L.J. 266 (1997) 607
Nemes, L., see Szalay, P.G. 263 (1996) 91
Nemoto, N., see Abe, J. 261 (1996) 18
Nemukhin, A.V., see Grigorenko, B.L. 270 (1997) 103
Neri, D., see Borghesani, A.F. 267 (1997) 116
Neria, E. and M. Karplus, Molecular dynamics of an enzyme reaction: proton transfer in TIM 267 (1997) 23
Nestmann, B., see Bündgen, P. 261 (1996) 625
Neuhauser, D., see Rom, N. 270 (1997) 382
Neuhauser, D., see Pang, J.W. 269 (1997) 392
Neumann, M.G., see Rivarola, C. 262 (1996) 131
Neumann, R. and N.C. Handy, Higher-order gradient corrections for exchange–correlation functionals 266 (1997) 16
Neusser, H.J., see Helm, R.M. 270 (1997) 285
Newport, R.J., see Walters, J.K. 264 (1997) 539
Newson, K.A. and S.D. Price, Isotope effects in the reaction of CF_2^{2+} with H_2/D_2 269 (1997) 93
Newton, M.A., see Hayden, B.E. 269 (1997) 485
Ng, C.F., see Au, C.T. 267 (1997) 44
Nguyen, M.T., see Lahem, D. 270 (1997) 93
Nguyen, M.T., see Sengupta, D. 265 (1997) 35
Nguyen, M.T., see Chandra, A.K. 268 (1997) 321
Nibu, Y., D. Sakamoto, T. Satho and H. Shimada, Dispersed phosphorescence spectra in a supersonic free jet by electric discharge excitation 262 (1996) 615
Niedner-Schatteburg, G., see Albert, G. 268 (1997) 235
Niesse, J.A. and H.R. Mayne, Minimization of small silicon clusters using the space-fixed modified genetic algorithm method 261 (1996) 576
Niikura, H., U. Graf and S. Hirayama, Intramolecular non-radiative relaxation from the first excited singlet background manifolds of anthracene and 9,10-dichloroanthracene in partially jet-cooled states 266 (1997) 217
Nikl, M., see Nagirnyi, V. 268 (1997) 280
Nikolaev, P., A. Thess, A.G. Rinzler, D.T. Colbert and R.E. Smalley, Diameter doubling of single-wall nanotubes 266 (1997) 422
Nikolaev, P., see Cowley, J.M. 265 (1997) 379
Nishi, N., see Ohashi, K. 263 (1996) 167
Nishi, N., see Inokuchi, Y. 269 (1997) 298
Nishikawa, M., see Holroyd, R.A. 266 (1997) 227
Nishimura, Y., see Tsuji, M. 262 (1996) 349
Nishimura, Y., see Tsuji, M. 266 (1997) 246

Nishino, N., see Oishi, O. 269 (1997) 530
Nishizawa, K., Y. Sakaguchi, H. Hayashi, H. Abe and G. Kido, A laser flash photolysis study of the effects of ultrahigh magnetic fields up to 29.6 T on dynamic behavior of radical pairs in micellar solutions 267 (1997) 501
Nisoli, M., see Lanzani, G. 264 (1997) 667
Nitsch, K., see Rodová, M. 268 (1997) 455
Nitzan, A., see Haran, A. 268 (1997) 475
Nizkorodov, S.A., Yu. Spinelli, E.J. Bieske, J.P. Maier and O. Dopfer, Dissociation energy of the Ar–HN_2^+ complex 265 (1997) 303
Nizkorodov, S.A., see Meuwly, M. 270 (1997) 252
Noack, F., see Radloff, W. 261 (1996) 301
Noack, F., see Radloff, W. 264 (1997) 210
Nobuto, T., see Miyasaka, H. 269 (1997) 281
Nocera, D.G., see Kim, J.U. 267 (1997) 323
Noga, J. and T. Pluta, Coupled cluster calculations of the electric properties of BeS. An analysis of the fifth-order non-iterative corrections 264 (1997) 101
Noga, J., see Tunega, D. 269 (1997) 435
Noguchi, H., S. Saito, S. Kidoaki and K. Yoshikawa, Self-organized nanostructures constructed with a single polymer chain 261 (1996) 527
Nomura, S. and Y. Shirota, Concentration dependence of the activation energy for the hole drift mobility of 9-ethylcarbazole-3-carbaldehyde diphenylhydrazone dispersed in polycarbonate 268 (1997) 461
Nomura, Y., see Ohkita, H. 263 (1996) 602
Nooijen, M., S.A. Perera and R.J. Bartlett, Partitioned equation-of-motion coupled cluster approach to indirect nuclear spin–spin coupling constants 266 (1997) 456
Noordam, L.D., see Maas, D.J. 270 (1997) 45
Noorman, J.T., see Gadd, G.E. 270 (1997) 108
Nord, S., see Ko, D.-S. 269 (1997) 54
Nordenskiöld, L., see van Dam, L. 262 (1996) 737
Nordlander, P., see Dutta, C.M. 264 (1997) 51
Nordlander, P., see Kim, S.G. 264 (1997) 345
Norimoto, M., see Nakashima, S. 268 (1997) 359
Norman, P., D. Jonsson and H. Ågren, Excited state properties through cubic response theory: polarizabilities of benzene and naphthalene 268 (1997) 337
Noro, T., H. Yamagishi and E. Miyoshi, A cluster model study for Li KVV transitions on a Cu (001) surface 261 (1996) 75
Noro, T., see Suzuki, Y. 268 (1997) 213
North, S.W. and G.E. Hall, The radical photodissociation channel of acrylonitrile 263 (1996) 148
Notario, R., O. Castaño and J.L.M. Abboud, Regarding the gas-phase acidity of CF_3OH 263 (1996) 367
Novoa, J.J. and F. Mota, Substituent effects in intermolecular $C(sp^3)$–$H \cdots O(sp^3)$ contacts: how strong can a $C(sp^3)$–$H \cdots O(sp^3)$ hydrogen bond be? 266 (1997) 23
Novoa, J.J., see Deumal, M. 265 (1997) 190
Novoa, J.J., see Perez del Valle, C. 269 (1997) 401
Novotny, L., see Bopp, M.A. 263 (1996) 721
Nowacki, J., see Herbich, J. 262 (1996) 633
Nowakowska, M., M. Smoluch and P. Petelenz, Mixing of exciton-transfer and charge-transfer contributions to the wavefunction of the naphthalene–hexachlorobiphenyl exciplex 270 (1997) 234

Nozaki, K., see Islam, A. 263 (1996) 209
Nyholm, R., see Andersen, J.N. 269 (1997) 371

Oberhammer, H., see Gobbato, K.I. 266 (1997) 527
Obi, K., see Ishiwata, T. 261 (1996) 175
Obi, K., see Mitsui, M. 262 (1996) 125
Ochoa de Aspuru, G., see Laganà, A. 267 (1997) 403
Ochsenfeld, C. and M. Head-Gordon, A reformulation of the coupled perturbed self-consistent field equations entirely within a local atomic orbital density matrix-based scheme 270 (1997) 399
Oesterhelt, D., see Hamm, P. 263 (1996) 613
Oesterhelt, D., see Hamm, P. 268 (1997) 180
Ogawa, T., see Tokeshi, M. 263 (1996) 783
Ogilvie, J.F., Comment on ''The adiabatic approximation'' 267 (1997) 590
Ogura, S., see Kohno, M. 267 (1997) 72
O'Halloran, M., see Dharmasena, K. 265 (1997) 308
Ohashi, K., Y. Inokuchi and N. Nishi, Pump–probe photodepletion spectroscopy of $(C_6H_6)_2^+$. Identification of spectrum in the charge resonance band region 263 (1996) 167
Ohashi, K., see Inokuchi, Y. 269 (1997) 298
Ohkita, H., Y. Nomura, A. Tsuchida and M. Yamamoto, Direct observation of the carbazole hole trap in polymer solid films by the charge-resonance band 263 (1996) 602
Ohnishi, A. and H. Kanno, Peculiar glass transition temperature rise with decreasing salt concentration in aqueous butyltripropylammonium chloride solution 263 (1996) 259
Ohno, M., see Oishi, O. 269 (1997) 530
Ohno, T., see Islam, A. 263 (1996) 209
Ohta, K., see Kamada, K. 263 (1996) 215
Ohta, K., see Kamada, K. 267 (1997) 402
Ohtani, H., see Kamiya, N. 265 (1997) 595
Oishi, O., S. Yamashita, M. Ohno, S. Lee, G. Sugihara and N. Nishino, Peculiar photophysical properties of a conformationally proximal pyrene-pair 269 (1997) 530
Okada, A., see Teki, Y. 270 (1997) 573
Okada, K., see Ibuki, T. 263 (1996) 173
Okada, S., see Kobayashi, T. 267 (1997) 472
Okada, T., see Imahori, H. 263 (1996) 545
Okada, T., see Katoh, R. 264 (1997) 631
O'Keeffe, F.J., see Ruth, A.A. 264 (1997) 605
Oki, S., see Egawa, C. 266 (1997) 169
Okuno, Y., Ab initio study of solvent kinetic isotope effects in microhydrated S_N2 reactions 264 (1997) 120
Okuyama, U., see Suzuki, T. 266 (1997) 107
Olexová, A., M. Melicherčík and L. Treindl, Oscillatory oxidation of Mn(II) ions by hexacyanoferrates(III) and bistability in the reduction of MnO_2 by hexacyanoferrates(II) in a CSTR 268 (1997) 505
Oleynikov, N.N., see Vertegel, A.A. 262 (1996) 455
Olsen, J., see Christiansen, O. 261 (1996) 369
Olsen, J., see Tokman, M. 265 (1997) 60
O'Malley, P.J., ^1H, ^{13}C and ^{17}O principal hyperfine tensor determination for the p-benzosemiquinone anion radical using hybrid density functional methods 262 (1996) 797
Ookubo, N., see Tomonari, M. 266 (1997) 488

Orel, A.E. and T.N. Rescigno, Photoionization of ammonia 269 (1997) 222
Orlandi, S., see Berardi, R. 261 (1996) 357
Orlovich, V.A., see Kruglik, S.G. 270 (1997) 293
Orozco, M. and F.J. Luque, Generalized linear response approximation in discrete methods 265 (1997) 473
Orr, B.J., see Payne, M.A. 265 (1997) 244
Orr-Ewing, A.J., see Wheeler, M.D. 268 (1997) 421
Osad'ko, I.S., M.A. Mikhailov and S.N. Gladenkova, Does the standard TLS model fail to explain the experimental data on the long-lived stimulated photon echo in amorphous solids? 270 (1997) 183
Osuka, A., see Kotani, S. 269 (1997) 274
Ottinger, Ch. and T. Winkler, Gateway coupling between quartet and doublet states of $^{15}N^{18}O$ studied in molecular beams 267 (1997) 294
Ottinger, Ch., see Mo, Y. 266 (1997) 267
Otto, C., see Kruglik, S.G. 270 (1997) 293
Ouchi, A., see Pola, J. 262 (1996) 279
Over, H., see Schwegmann, S. 264 (1997) 680
Ozanne, L., J.M. Hartmann, J.P. Bouanich and C. Boulet, Collisional narrowing of gas phase infrared bands of CO_2 at high density 261 (1996) 353

Paddon-Row, M.N., see Bell, T.D.M. 268 (1997) 223
Padhye, S., see Swarnabala, G. 267 (1997) 539
Pagsberg, P., see Meunier, H. 261 (1996) 277
Palese, S., see Kumble, R. 261 (1996) 396
Palit, D.K., A.V. Sapre and J.P. Mittal, Picosecond studies on the electron transfer from pyrene and perylene excited singlet states to N-hexadecyl pyridinium chloride 269 (1997) 286
Palit, D.K., see Ghosh, H.N. 265 (1997) 365
Palm, H. and F. Merkt, Ion density effects in the pulsed field ionization of high Rydberg states 270 (1997) 1
Palma, J. and J. Echave, An analytical Fourier transform method for semiclassical quantization 270 (1997) 206
Palmer, P.M., see Andrews, P.M. 265 (1997) 224
Palmer, P.M., see Pryor, B.A. 267 (1997) 531
Palomar, J., see Catalán, J. 269 (1997) 151
Pampel, A., see Volke, F. 262 (1996) 374
Panas, I. and R. Gatt, How repulsive are holes to local antiferromagnetic order in cuprates? 266 (1997) 410
Panas, I. and R. Gatt, On the superconductivity in $(Sr, Ca)_{14}Cu_{24}O_{41}$ – towards a chemical standard model 270 (1997) 178
Pang, J.W. and D. Neuhauser, Application of generalized filter-diagonalization to extract instantaneous normal modes (Chem. Phys. Letters 252 (1996) 173). Erratum 269 (1997) 392
Pang, X.Y., see Feng, W.L. 266 (1997) 43
Pang, Z., see Masoumi, Z. 261 (1996) 551
Pant, D., see Neelakandan, M. 265 (1997) 283
Paolucci, G., see Comelli, G. 261 (1996) 253
Paolucci, G., see Polzonetti, G. 267 (1997) 384
Papaconstantopoulos, D.A., see Li, Y. 268 (1997) 331
Papagiannakopoulos, P., see Kambanis, K.G. 261 (1996) 457
Papagiannakopoulos, P., see Kambanis, K.G. 268 (1997) 498
Pápai, I. and M. Castro, A density functional study of Sc_2 and Sc_3 267 (1997) 551

Papanikolas, J.M., see Williams, R.M. 261 (1996) 405
Park, S.C., see Lee, T.G. 264 (1997) 303
Parmon, V.N., see Makarshin, L.L. 266 (1997) 173
Parr, R.G., see Wang, Y.A. 267 (1997) 14
Parry, D.E., see Jeffreys, N. 266 (1997) 537
Parry, D.E., see Silcocks, S.E. 262 (1996) 355
Parson, R., see Faeder, J. 270 (1997) 196
Parson, R., see Maslen, P.E. 263 (1996) 63
Parson, W.W., see Warshel, A. 265 (1997) 293
Pascual, J.L. and L.G.M. Pettersson, Electrostatic potential from embedded clusters 270 (1997) 351
Pastawski, H.M., G. Usaj and P.R. Levstein, Quantum interference phenomena in the local polarization dynamics of mesoscopic systems: an NMR observation 261 (1996) 329
Pasterny, K., see Gwóźdź, E. 267 (1997) 557
Pate, M.A., see Lidzey, D.G. 263 (1996) 655
Patzelt, H., see Hamm, P. 263 (1996) 613
Patzelt, H., see Hamm, P. 268 (1997) 180
Pavese, M., see Calhoun, A. 262 (1996) 415
Payne, M.A., A.P. Milce, M.J. Frost and B.J. Orr, Dynamical symmetry breaking in the $4\nu_{CH}$ rovibrational manifold of acetylene 265 (1997) 244
Payne, M.G., see Deng, L. 270 (1997) 299
Pazé, C., see Lamberti, C. 269 (1997) 500
Pazyuk, E.A., A.V. Stolyarov and V.I. Pupyshev, Improvement on Van Vleck's formula for diatomic nonadiabatic energy shifts 267 (1997) 207
Pazzi, G.P., see Nagirnyi, V. 268 (1997) 280
Pearlstein, R.M., Antenna exciton trapping kinetics as a probe of primary electron transfer heterogeneity in the photosynthetic reaction center 262 (1996) 442
Pearson, J., see Ashfold, M.N.R. 263 (1996) 138
Peden, C.H.F., see Chambers, S.A. 267 (1997) 51
Pederson, M.R., see Rencsok, R. 262 (1996) 207
Pédrini, C., see Zhang, L. 268 (1997) 408
Pedron, D., see Mulloni, V. 263 (1996) 331
Peel, J.B., see Khairallah, G. 268 (1997) 218
Peeters, J., see Devriendt, K. 261 (1996) 450
Pellaux, R., see Hauser, A. 261 (1996) 313
Pelupessy, P., see Fu, R. 264 (1997) 63
Peng, J., see Dianxun, W. 262 (1996) 771
Peng, T., see Kouri, D.J. 262 (1996) 519
Penner, G.H., Simultaneous determination of the lithium-6 nuclear quadrupolar coupling constant and chemical shift anisotropy in monomeric tri(isopropyl)phenyllithium 261 (1996) 665
Perchard, J.P., see Asselin, P. 268 (1997) 265
Perdew, J.P., see Burke, K. 265 (1997) 115
Pereira, C.M., W. Schmickler, A.F. Silva and M.J. Sousa, On the capacity of liquid–liquid interfaces 268 (1997) 13
Perera, L., see Yeh, I.-C. 264 (1997) 31
Perera, S.A., see Nooijen, M. 266 (1997) 456
Pérez, P., R. Contreras, A. Vela and O. Tapia, Relationship between the electronic chemical potential and proton transfer barriers 269 (1997) 419

Perez del Valle, C. and J.J. Novoa, Density functional computations on the structure and stability of $OH^-(H_2O)_n$ ($n = 1–3$) clusters. A test study 269 (1997) 401
Persico, M., see Magnier, S. 262 (1996) 747
Person, W.B., see Del Bene, J.E. 264 (1997) 109
Persoons, A., see Hendrickx, E. 270 (1997) 241
Petelenz, P., see Nowakowska, M. 270 (1997) 234
Peterman, E.J.G., R. Monshouwer, I.H.M. van Stokkum, R. van Grondelle and H. van Amerongen, Ultrafast singlet excitation transfer from carotenoids to chlorophylls via different pathways in light-harvesting complex II of higher plants 264 (1997) 279
Petrosyan, A., see Zhang, L. 268 (1997) 408
Pettersson, J.B.C., see Svanberg, M. 263 (1996) 661
Pettersson, L.G.M., see Pascual, J.L. 270 (1997) 351
Peyerimhoff, S.D., see Sumathi, R. 263 (1996) 742
Pfeiffer, M., A. Lau, K. Lenz and T. Elsaesser, Anharmonicity effects in the resonance Raman spectra of heterocyclic aromatic molecules showing photoinduced intramolecular proton transfer 268 (1997) 258
Pfeiffer, M., see Chudoba, C. 263 (1996) 622
Pfeiffer, M., see Lau, A. 263 (1996) 435
Pfeiffer, M., see Werncke, W. 266 (1997) 99
Pflumio, V., see Miranda, P.B. 264 (1997) 387
Phillips, A.J., see Hamilton, P.A. 264 (1997) 245
Phillips, D., see Henari, F.Z. 267 (1997) 229
Phillips, D., see Scholes, G.D. 266 (1997) 521
Phillips, D.L., see Kwok, W.M. 261 (1996) 685
Phillips, D.L., see Kwok, W.M. 262 (1996) 699
Phillips, D.L., see Kwok, W.M. 270 (1997) 506
Phillips, L.F., Velocity and angular distributions of molecules emitted from a liquid surface 266 (1997) 161
Piet, J.J., J.M. Warman and H.L. Anderson, Photo-induced charge separation on conjugated porphyrin chains 266 (1997) 70
Pietzak, B., C. Wolf, H.J. Möckel and A. Weidinger, Influence of oxygen on the production of higher fullerenes 265 (1997) 200
Pimenov, A.V., see Argyrakis, P. 268 (1997) 372
Pinot de Moira, J.C., see Ball, S.M. 264 (1997) 531
Pirani, F., see de Castro Vítores, M. 263 (1996) 456
Pircher, P., see Li, X. 263 (1996) 463
Piryatinski, A. and R.T. Deck, Excimer states and enhanced two-photon absorption in intramolecular charge-transfer crystals 269 (1997) 156
Pisarski, W.A., see Ryba-Romanowski, W. 264 (1997) 323
Piseri, P., see Biasioli, F. 270 (1997) 115
Piślewski, N., see Tritt-Goc, J. 268 (1997) 471
Pizio, O., see Trokhymchuk, A. 262 (1996) 33
Plakhotnik, T., D. Walser, A. Renn and U.P. Wild, Two Shpol'skii sites of all-trans-1,8-diphenyloctatetraene in n-tetradecane 262 (1996) 379
Plakhotnik, T., see Walser, D. 270 (1997) 16
Plank, R.V., Y. Wei, N.J. DiNardo and J.M. Vohs, Characterization of highly conducting, ultra-thin polyaniline films produced by evaporative deposition 263 (1996) 33
Plaza, P., see Meyer, Y.H. 264 (1997) 643
Pluta, T., see Noga, J. 264 (1997) 101

Podsiadła, D., see Ryba-Romanowski, W. 264 (1997) 323
Pohl, R., see Yamazaki, T. 265 (1997) 137
Poirier, B. and W.H. Miller, Optimized preconditioners for Green function evaluation in quantum reactive scattering calculations 265 (1997) 77
Pola, J., A. Ouchi, K. Saito, K. Ishikawa and Y. Koga, Efficient chemical vapour deposition of hydrocarbon polymeric films by UV laser induced photolysis of 3-butyn-2-one 262 (1996) 279
Polisset-Thfoin, M., see Diamy, A.-M. 269 (1997) 327
Polzonetti, G., G. Iucci, C. Furlani, M.V. Russo, A. Furlani, G. Infante, G. Paolucci, B. Brena and D. Cocco, A photoelectron spectroscopic study of the interface formation between chromium and a palladium-intercalated polymer film 267 (1997) 384
Pope, P.E., see Hain, T.D. 262 (1996) 723
Pople, J.A., see Curtiss, L.A. 270 (1997) 419
Popovič, D.B., see Allan, M. 268 (1997) 50
Popp, J., see Trunk, M. 264 (1997) 233
Porezag, D., see Seifert, G. 268 (1997) 352
Port, H., see Gómez, U. 268 (1997) 1
Porto, A.O., W.F. Magalhães and J.C. Machado, Inhibition of positronium formation and its quenching reactions in binary solid solutions and mixtures of metal tris-2,2,6,6-tetramethyl-3,5-heptanedionate (dpm) complexes 266 (1997) 329
Poulet, G., see Bedjanian, Y. 266 (1997) 233
Prandolini, M.J., see Ball, G.E. 261 (1996) 421
Prasad, P., see Gadd, G.E. 270 (1997) 108
Prekas, D., see Lüder, C. 267 (1997) 149
Previtali, C.M., see Rivarola, C. 262 (1996) 131
Pribble, R.N., C. Gruenloh and T.S. Zwier, The ultraviolet and infrared spectroscopy of $(benzene)_2$–$(CH_3OH)_3$ isomeric clusters 262 (1996) 627
Price, P., see Harima, Y. 262 (1996) 274
Price, S.D., see Newson, K.A. 269 (1997) 93
Price, S.L., see Coombes, D.S. 265 (1997) 532
Pryor, B.A., P.M. Andrews, P.M. Palmer and M.R. Topp, Perylene complexes with *p*-dichlorobenzene and related species: comparison of rotational coherence data with structure calculations 267 (1997) 531
Pryor, B.A., see Andrews, P.M. 265 (1997) 224
Pucci, D., see Ghedini, M. 267 (1997) 341
Pupyshev, V.I., see Pazyuk, E.A. 267 (1997) 207
Purchase, R.L., see Fischer, G. 262 (1996) 689
Pyykkö, P., see Tokman, M. 265 (1997) 60

Qi, X., H.G. Gallagher, T.P.J. Han, B. Henderson, R. Illingworth and I.S. Ruddock, Laser heated pedestal growth and spectroscopic properties of $K_2NdNb_5O_{15}$ and Ba_2NdNbO_6 crystals 264 (1997) 623
Qian, X., see Wang, D. 266 (1997) 560
Qin, L.-C. and S. Iijima, Onion-like graphitic particles produced from diamond 262 (1996) 252
Qin, L.-C. and S. Iijima, Structure and formation of raft-like bundles of single-walled helical carbon nanotubes produced by laser evaporation 269 (1997) 65
Qin, L.-C., S. Iijima, H. Kataura, Y. Maniwa, S. Suzuki and Y. Achiba, Helicity and packing of single-walled carbon nanotubes studied by electron nanodiffraction 268 (1997) 101

Qiu, F., X. Cheng, K. Misawa and T. Kobayashi, Multiple reflection correction in the determination of the complex electro-optic constant using a Mach-Zehnder interferometer 266 (1997) 153
Qiyuan, Z., see Dianxun, W. 262 (1996) 771
Quack, M., U. Schmitt and M.A. Suhm, FTIR spectroscopy of hydrogen fluoride clusters in synchronously pulsed supersonic jets. Isotopic isolation, substitution and 3-d condensation 269 (1997) 29
Quack, M., see Klopper, W. 261 (1996) 35
Quitevis, E.L., see Neelakandan, M. 265 (1997) 283
Quitevis, E.L., see Sengupta, A. 263 (1996) 25
Qureshi, R.A., see Khan, M.A. 264 (1997) 273

Radi, P.P., H.-M. Frey, B. Mischler, A.P. Tzannis, P. Beaud and T. Gerber, Stimulated emission pumping of OH and NH in flames by using two-color resonant four-wave mixing 265 (1997) 271
Radloff, W., Th. Freudenberg, H.-H. Ritze, V. Stert, F. Noack and I.V. Hertel, Lifetime of the benzene dimer in the S_2 electronic state 261 (1996) 301
Radloff, W., Th. Freudenberg, V. Stert, H.-H. Ritze, F. Noack and I.V. Hertel, Cluster size dependence of the internal conversion in highly excited benzene$(NH_3)_n$ clusters 264 (1997) 210
Radloff, W., see Freudenberg, Th. 269 (1997) 523
Radom, L., see Gauld, J.W. 262 (1996) 187
Raghavachari, K., see Curtiss, L.A. 270 (1997) 419
Raghunathan, P., see Ilangovan, U. 263 (1996) 223
Rahman, N., The degenerate two-level system and high-order harmonic generation 270 (1997) 189
Rahman, N., see Magnier, S. 262 (1996) 747
Raitsimring, A. and P. Borbat, Electron spin-echo modulation for a '1 + 2' pulse train in a weak hyperfine interaction limit 262 (1996) 8
Rajasekharan, M.V., see Swarnabala, G. 267 (1997) 539
Raj Gopal, V., V. Jayathirtha Rao, G. Saroja and A. Samanta, Photophysical behaviour of some pyrenylethylene derivatives and its implication on trans → cis photoisomerisation reactions 270 (1997) 593
Rakestraw, D.J., see Scherer, J.J. 265 (1997) 169
Rakhmanina, A.V., see Agafonov, V. 267 (1997) 193
Rakitzis, T.P., see Kandel, S.A. 265 (1997) 121
Ramachandran, B., J. Senekowitsch and R.E. Wyatt, A quasiclassical trajectory study of the reaction $O(^3P) + HCl\ (v = 2,\ j = 1, 6, 9) \rightarrow OH(v',\ j') + Cl$ on a new potential surface 270 (1997) 387
Ramasami, T., see Subramanian, V. 264 (1997) 92
Ranasinghe, M.G., see Bell, T.D.M. 268 (1997) 223
Randriamanantenasoa, Z., see Diamy, A.-M. 269 (1997) 327
Rantala, T.T., see Hyvönen, M. 268 (1997) 55
Rao, C.N.R., see Sen, R. 267 (1997) 276
Rappuoli, R., see Rossi, C. 264 (1997) 205
Rapta, P., see Staško, A. 262 (1996) 233
Räther, G., see Mayer, I. 270 (1997) 211
Rathje, J., see Williams, R.M. 261 (1996) 405
Rauw, W., see Hazenkamp, M.F. 265 (1997) 264

Ravichandran, K., Y. Bai and T.R. Fletcher, Techniques for stimulated Raman excitation and CARS detection of radicals created by photodissociation 261 (1996) 261
Ravikanth, M., see Sevian, A. 263 (1996) 241
Ravindra Kumar, G., see Vijayalakshmi, K. 270 (1997) 37
Ravishankara, A.R., see Rudich, Y. 261 (1996) 467
Ravishankara, A.R., see Talukdar, R.K. 262 (1996) 669
Rayane, D., see Antoine, R. 261 (1996) 670
Read, J.P. and A.D. Buckingham, Comment on: "The ν_3 infrared spectrum of the $He–NH_4^+$ complex" 270 (1997) 245
Rebane, A., D. Reiss, I. Renge and U.P. Wild, Non-destructive readout of picosecond time-and-space-domain holograms recorded by photon-gated spectral hole burning 262 (1996) 155
Reddic, J.E. and M.A. Duncan, Composite samples and the generation of novel metal carbide clusters 264 (1997) 157
Reddy, B.V., see Reuse, F.A. 267 (1997) 258
Redfern, P.C., see Curtiss, L.A. 270 (1997) 419
Redlich, Ph., see Banhart, F. 269 (1997) 349
Reguero, M., R. Caballol, J.-L. Heully and J.-P. Malrieu, Calculation of small transition energies from a dressed configuration interaction 265 (1997) 621
Reid, J.P., P.W. Barnes and C.J.S.M. Simpson, The influence of the attractive well on near and non-resonant vibrational energy transfer in the gas phase: CO($v = 1$) deactivated by methane deuteroisomers 268 (1997) 150
Reinen, D., see Hazenkamp, M.F. 265 (1997) 264
Reininger, R., see Altmann, K.N. 261 (1996) 597
Reiss, D., see Rebane, A. 262 (1996) 155
Remko, M., K.R. Liedl and B.M. Rode, Gas-phase acidities of HM(=X)XH (M = C, Si; X = O, S) acids calculated by ab initio molecular orbital methods at the G2 level of theory 263 (1996) 379
Remko, M., Gas-phase binding of Li^+, Na^+ and Mg^{2+} to formaldehyde, acetaldehyde and their silicon and sulfur analogs. A theoretical study by means of ab initio molecular orbital methods at the G2 level of theory 270 (1997) 369
Remmers, M., see Gelinck, G.H. 265 (1997) 320
Rempe, S.B. and R.O. Watts, The convergence properties of hindered rotor energy levels 269 (1997) 455
Rencsok, R., K.A. Jackson, T.A. Kaplan, J.F. Harrison and M.R. Pederson, Electronic properties of the electride-type molecule Li(9-crown-3)$_2$. Comparison of Hartree–Fock and local density approximations: implications for crystalline crown ether electrides 262 (1996) 207
Rendell, A.P., see Kobayashi, R. 265 (1997) 1
Renge, I., see Rebane, A. 262 (1996) 155
Renn, A., see Bach, H. 266 (1997) 317
Renn, A., see Plakhotnik, T. 262 (1996) 379
Renn, A., see Walser, D. 270 (1997) 16
Rérat, M. and A. Lichanot, Compton profiles of the isoelectronic BeO and BN molecules: an ab initio study 263 (1996) 767
Rescigno, T.N., see Orel, A.E. 269 (1997) 222
Resnyanskii, E.D., A.V. Myshlyavtsev, V.I. Elokhin and B.S. Bal'zhinimaev, Dissociative adsorption on rough surfaces with dynamically changing morphology: a Monte Carlo model 264 (1997) 174
Rettig, W., see Braun, D. 268 (1997) 110

Reuse, F.A., S.N. Khanna, B.V. Reddy and J. Buttet, N_2 adsorption around small Ni_n ($n = 2$–4) clusters 267 (1997) 258
Reynhardt, E.C. and C.J. Terblanche, ^{13}C relaxation in natural diamond 269 (1997) 464
Reynolds, C.A., see Mura, M.E. 262 (1996) 533
Reynolds, G. and E.A. Carter, Removal of the bottleneck in local correlation methods 265 (1997) 660
Rhee, Y.M., see Lee, T.G. 264 (1997) 303
Richards, P.L., see Grannan, S.M. 264 (1997) 359
Richter, R.C., see Silvente, E. 264 (1997) 309
Riedle, E., see Chudoba, C. 263 (1996) 622
Riesen, H., see Hauser, A. 261 (1996) 313
Rigden, J.S., see Walters, J.K. 264 (1997) 539
Rikken, G.L.J.A., see Verbandt, Y. 270 (1997) 471
Ringling, J., see Freudenberg, Th. 269 (1997) 523
Rinzler, A.G., see Nikolaev, P. 266 (1997) 422
Ritze, H.-H., see Radloff, W. 261 (1996) 301
Ritze, H.-H., see Radloff, W. 264 (1997) 210
Rivail, J.-L., see Assfeld, X. 263 (1996) 100
Rivarola, C., S.G. Bertolotti, C.D. Borsarelli, J.J. Cosa, C.M. Previtali and M.G. Neumann, Hydrogen bonding and charge transfer interactions in exciplexes formed by excited indole and monosubstituted benzenes in cyclohexane 262 (1996) 131
Robbe, J.M., H. Lavendy, J.P. Flament and G. Chambaud, Ro-vibronic spectrum of the HCSi radical 267 (1997) 91
Robinson, B.H., see Duffy, N.W. 266 (1997) 451
Rocca, M., see Åkerlund, C. 270 (1997) 157
Rocca, M., see Buatier de Mongeot, F. 270 (1997) 345
Rocchi, C., see Bizzarri, A.R. 263 (1996) 559
Rode, B.M., see Remko, M. 263 (1996) 379
Rodger, P.M., see Westacott, R.E. 262 (1996) 47
Rodham, D.A. and G.A. Blake, ZEKE-PFI spectroscopy of 1:1 complexes of sodium with water and ammonia 264 (1997) 522
Rodová, M., A. Cihlář, Z. Málková and K. Nitsch, New differential thermal analysis study of lead halides 268 (1997) 455
Rodriguez, J.A., see Hrbek, J. 267 (1997) 65
Roeselová, M., see Nachtigallová, D. 270 (1997) 357
Rohlfing, E.A., see Tobiason, J.D. 261 (1996) 387
Rollins, H.W., R. Dabestani and Y.-P. Sun, Spectroscopic investigations of intramolecular and intermolecular excimers of 1,3-di(2-naphthyl)propane and methylnaphthalenes in supercritical carbon dioxide 268 (1997) 187
Rom, N., D.M. Charutz and D. Neuhauser, Shifted-contour auxiliary-field Monte Carlo: circumventing the sign difficulty for electronic-structure calculations 270 (1997) 382
Romanini, D., A.A. Kachanov and F. Stoeckel, Cavity ringdown spectroscopy: broad band absolute absorption measurements 270 (1997) 546
Romanini, D., A.A. Kachanov and F. Stoeckel, Diode laser cavity ring down spectroscopy 270 (1997) 538
Romanini, D., A.A. Kachanov, N. Sadeghi and F. Stoeckel, CW cavity ring down spectroscopy 264 (1997) 316
Romero, T., J. de Andrés, M. Albertí, J.M. Lucas, J. Rubio, J.P. Daudey and A. Aguilar, Adiabatic and diabatic representations of potential energy curves for the $(NaRb)^+$ system 261 (1996) 583

Rommens, J., see Chattopadhyay, N. 264 (1997) 265
Roney, A., C.J. Delisle and M. Larzillière, Measurements of kinetic energies released to the $2s\ ^3S + 1s\ ^1S$ dissociation threshold of He_2 270 (1997) 59
Rosato, A., see Bertini, I. 265 (1997) 677
Röschinger, T., see Hamm, P. 263 (1996) 613
Röschinger, T., see Hamm, P. 268 (1997) 180
Rosei, R., see Comelli, G. 261 (1996) 253
Rosén, A., see Grönbeck, H. 264 (1997) 39
Rosenblum, G., D. Grosswasser, F. Schael, M.B. Rubin and S. Speiser, Electronic energy transfer in supersonic jet expanded naphthalene–$(CH_2)_n$–anthracene bichromophoric molecules 263 (1996) 441
Rosenwaks, S., see Arusi-Parpar, T. 268 (1997) 163
Rospenk, M., A. Koll and L. Sobczyk, Proton transfer and secondary deuterium isotope effect in the ^{13}C NMR spectra of ortho-aminomethyl phenols 261 (1996) 283
Rossi, C., A. Donati, C. Bonechi, G. Corbini, R. Rappuoli, E. Dreassi and P. Corti, Nuclear relaxation studies in ligand–macromolecule affinity index determinations 264 (1997) 205
Rossi, G., see Soriano, L. 266 (1997) 184
Rossi, M.L., see Brivio, G.P. 263 (1996) 597
Roszak, S. and K. Balasubramanian, Theoretical study of the isomerization of $TaC_n^+ (n = 7–13)$ cations 265 (1997) 553
Roszak, S. and K. Balasubramanian, Stabilities of isomers of LaC_{12}^+ and LaC_{13}^+ 264 (1997) 80
Roteta, M., see García, G. 264 (1997) 589
Roth, W., see Schumm, S. 263 (1996) 126
Rowe, B.R., see Le Garrec, J.L. 270 (1997) 66
Rowland, B. and W.P. Hess, The ultraviolet photochemistry of condensed-phase acetyl chloride 263 (1996) 574
Rubin, M.B., see Rosenblum, G. 263 (1996) 441
Rubio, J., see Romero, T. 261 (1996) 583
Rübsam, M., P. Schweitzer and K.-P. Dinse, Nuclear quadrupole interaction in $Sc@C_{82}$ 263 (1996) 540
Ruddock, I.S., see Qi, X. 264 (1997) 623
Rudich, Y., R.K. Talukdar, T. Imamura, R.W. Fox and A.R. Ravishankara, Uptake of NO_3 on KI solutions: rate coefficient for the $NO_3 + I^-$ reaction and gas-phase diffusion coefficients for NO_3 261 (1996) 467
Rüdiger, W., see Teuchner, K. 268 (1997) 157
Ruiz, A., J. Bretón and J.M. Gomez Llorente, Scattering cross sections for low-energy rage-gas + C_{60} and $C_{60} + C_{60}$ collisions 270 (1997) 121
Ruland, H., see Bürger, H. 268 (1997) 249
Ruoff, P., see Treindl, L. 269 (1997) 263
Ruppe, H., see Heufelder, J. 269 (1997) 1
Russell, T.P., T.M. Allen and Y.M. Gupta, Time resolved optical spectroscopy to examine chemical decomposition of energetic materials under static high pressure and pulsed heating conditions 267 (1997) 351
Russo, M.V., see Polzonetti, G. 267 (1997) 384
Rustici, M., M. Branca, C. Caravati and N. Marchettini, Evidence of a chaotic transient in a closed unstirred cerium catalyzed Belousov–Zhabotinsky system 263 (1996) 429
Ruth, A.A. and M.T. Wick, The $S_0 \rightarrow S_4$ transition of jet-cooled fluoranthene: vibronic coupling of S_4 with S_3 266 (1997) 206

Ruth, A.A., F.J. O'Keeffe, M.W.D. Mansfield and R.P. Brint, The resonance-enhanced multiphoton excitation spectrum of jet-cooled 4-H-1-benzopyrane-4-thione 264 (1997) 605
Rutherford, A.W., see Deligiannakis, Y. 270 (1997) 564
Rutz, S. and E. Schreiber, Fractional revivals of wave packets in the $A^1\Sigma_u^+$ state of K_2. A comparison of two different pump and probe cycles by spectrograms 269 (1997) 9
Rutz, S., see Heufelder, J. 269 (1997) 1
Ruud, K. and T. Helgaker, The magnetizability, rotational *g* tensor, and quadrupole moment of PF_3 revisited 264 (1997) 17
Ryba-Romanowski, W., S. Gołąb, W.A. Pisarski, D. Podsiadła and Z. Czapla, Optical spectroscopy of a chromium doped $(CH_3)_2NH_2Al(SO_4)_2 \cdot 6H_2O$ single crystal in the ferroelectric phase 264 (1997) 323

Saalfrank, P., see Finger, K. 268 (1997) 291
Saam, B., N. Drukker and W. Happer, Edge enhancement observed with hyperpolarized ^3He 263 (1996) 481
Sabo, D., Z. Bačić, S. Graf and S. Leutwyler, Three-dimensional model treatment of the torsional levels of isotopic water trimers 261 (1996) 318
Sadeghi, N., see Zikratov, G. 265 (1997) 585
Sadeghi, N., see Romanini, D. 264 (1997) 316
Sadílek, M. and F. Tureček, Laser photolysis of $ND_4^{\cdot}$ and trimethylamine formed by collisional neutralization of their cations in the gas phase 263 (1996) 203
Sáez Rábanos, V., see Aoiz, F.J. 262 (1996) 175
Sáez Rábanos, V., see Aoiz, F.J. 264 (1997) 487
Safvan, C.P., see Vijayalakshmi, K. 270 (1997) 37
Sagdeev, R.Z., see Bagryanskaya, E.G. 264 (1997) 655
Saijo, H., see Miranda, P.B. 264 (1997) 387
Saik, V.O. and S. Lipsky, Magnetic field effects on recombination fluorescence: comparison of VUV and fast electron excitation 264 (1997) 649
Saito, K., see Pola, J. 262 (1996) 279
Saito, S., see Noguchi, H. 261 (1996) 527
Saitow, K., Y. Naitoh, K. Tominaga and K. Yoshihara, Photo-induced reactions of CH_2I_2 in solution studied by the ultrafast transient absorption spectroscopy 262 (1996) 621
Saitow, K.-i., see Inokuchi, Y. 269 (1997) 298
Sakaguchi, T., see Kamada, K. 263 (1996) 215
Sakaguchi, T., see Kamada, K. 267 (1997) 402
Sakaguchi, Y., see Nishizawa, K. 267 (1997) 501
Sakamoto, D., see Nibu, Y. 262 (1996) 615
Sakata, Y., see Imahori, H. 263 (1996) 545
Sakata, Y., see Zhao, X. 262 (1996) 643
Sako, T. and K. Yamanouchi, Algebraic approach to vibrationally highly excited states of SO_2. Vibrational wavefunctions from spectroscopy 264 (1997) 403
Sakuragi, H., see Waga, M. 265 (1997) 277
Salahub, D.R., see Malkin, V.G. 261 (1996) 335
Salikhov, K.M., D.J. Schneider, S. Saxena and J.H. Freed, A theoretical approach to the analysis of arbitrary pulses in magnetic resonance (Chem. Phys. Letters 262 (1996) 17). Erratum 265 (1997) 562
Salikhov, K.M., D.J. Schneider, S. Saxena and J.H. Freed, A theoretical approach to the analysis of arbitrary pulses in magnetic resonance 262 (1996) 17

Salikhov, K.M., see Dvinskikh, S.V. 268 (1997) 401
Saltzman, E.S., see Silvente, E. 264 (1997) 309
Salvalaggio, M., see Lamberti, C. 269 (1997) 500
Salvi, P.R., see Gellini, C. 268 (1997) 381
Samanta, A., see Raj Gopal, V. 270 (1997) 593
Sameshima, Y., see Kurawaki, J. 266 (1997) 353
Samulski, E.T., see Terzis, A.F. 264 (1997) 481
Sánchez Rayo, M.N., see Fernández, J.A. 267 (1997) 301
Sander, W., see Kraka, E. 268 (1997) 313
Sanderson, A., see Holmes, A.S. 266 (1997) 309
Sandilands, D.W.D., see Moazzen-Ahmadi, N. 265 (1997) 563
Sanker, S., see Subramanian, V. 264 (1997) 92
Santamaría, J., see Muñoz-Crego, C. 261 (1996) 569
Sanz, J.M., see Soriano, L. 266 (1997) 184
Sapre, A.V., see Ghosh, H.N. 265 (1997) 365
Sapre, A.V., see Palit, D.K. 269 (1997) 286
Saroja, G., see Raj Gopal, V. 270 (1997) 593
Sasaki, F., see Suzuki, Y. 268 (1997) 213
Sassara, A., G. Zerza and M. Chergui, Phosphorescence of C_{60} in rare gas matrices 261 (1996) 213
Sassenberg, U., see Doverstål, M. 270 (1997) 273
Sastre, G., P.M. Viruela and A. Corma, Quantum chemistry calculations on the effect of electron confinement upon the frontier molecular orbitals of ethylene and benzene in sodalite. Implications on reactivity 264 (1997) 565
Satho, T., see Nibu, Y. 262 (1996) 615
Sathyamurthy, N., see Chakrabarti, N. 267 (1997) 31
Sato, K., see Kohno, M. 267 (1997) 72
Sato, S., see Verma, A.L. 267 (1997) 507
Sato, S., see Vondrák, T. 261 (1996) 481
Saue, T., K. Faegri and O. Gropen, Relativistic effects on the bonding of heavy and superheavy hydrogen halides 263 (1996) 360
Sauer, J., see Haase, F. 266 (1997) 397
Sauer, J., see Stein, M. 267 (1997) 111
Sauer, M., see Müller, R. 262 (1996) 716
Sauer, M., see Ko, D.-S. 269 (1997) 54
Sauer, T., see Janke, W. 263 (1996) 488
Saxena, S., see Salikhov, K.M. 262 (1996) 17
Saxena, S., see Salikhov, K.M. 265 (1997) 562
Scarano, D., see Lamberti, C. 269 (1997) 500
Schaaff, T.G., see Alvarez, M.M. 266 (1997) 91
Schael, F., see Rosenblum, G. 263 (1996) 441
Schafer, O., see Daul, C. 262 (1996) 74
Schäfer, W., see Limantara, L. 262 (1996) 656
Schaldach, C.M., see Wilson, W.D. 267 (1997) 431
Schatz, G.C., see Takayanagi, T. 265 (1997) 410
Scheblykin, I.G., M.A. Drobizhev, O.P. Varnavsky, M. Van der Auweraer and A.G. Vitukhnovsky, Reorientation of transition dipoles during exciton relaxation in J-aggregates probed by fluorescence anisotropy 261 (1996) 181
Scheer, H., see Limantara, L. 262 (1996) 656

Scheffler, M., see Gross, A. 263 (1996) 567
Scheier, P., see Senn, G. 266 (1997) 276
Scheier, P., see Matt, S. 264 (1997) 149
Scheiner, S., see Yi, M. 262 (1996) 567
Scheler, U. and R.K. Harris, Fluorine-19 NMR of solids with both homonuclear (multi-pulse) decoupling and pulsed proton decoupling 262 (1996) 137
Scherer, J.J. and D.J. Rakestraw, Cavity ringdown laser absorption spectroscopy detection of formyl (HCO) radical in a low pressure flame 265 (1997) 169
Scherer, N.F., see Wang, W. 262 (1996) 573
Scherer, P.O.J. and S.F. Fischer, Interpretation of a low-lying excited state of the reaction center of *Rb. sphaeroides* as a double triplet 268 (1997) 133
Schettino, V., see Gellini, C. 268 (1997) 381
Schiedt, J. and R. Weinkauf, Photodetachment photoelectron spectroscopy of mass selected anions: anthracene and the anthracene–H_2O cluster 266 (1997) 201
Schikarski, T., see Fuß, W. 262 (1996) 675
Schlag, E.W., see Der Chao, S. 265 (1997) 445
Schlag, E.W., see Held, A. 267 (1997) 318
Schlegel, H.B., see Wittbrodt, J.M. 265 (1997) 527
Schlegel, H.B., see Wittbrodt, J.M. 269 (1997) 391
Schleyer, P. von R., see Urban, J. 264 (1997) 441
Schmickler, W., see Pereira, C.M. 268 (1997) 13
Schmid, G., see Smith, B.A. 270 (1997) 139
Schmid, R.P., see Arusi-Parpar, T. 268 (1997) 163
Schmid, W.E., see Fuß, W. 262 (1996) 675
Schmidt, M., see Cummins, T.R. 261 (1996) 228
Schmidt, R. and M. Schütz, Determination of reaction volumes and reaction enthalpies by photoacoustic calorimetry 263 (1996) 795
Schmidt, R., see Yamazaki, T. 265 (1997) 137
Schmidt, S.J., see Soos, Z.G. 265 (1997) 427
Schmitt, M., G. Knopp, A. Materny and W. Kiefer, Femtosecond time-resolved coherent anti-Stokes Raman scattering for the simultaneous study of ultrafast ground and excited state dynamics: iodine vapour 270 (1997) 9
Schmitt, U., see Quack, M. 269 (1997) 29
Schmitz-Huebsch, Th., see Grummt, U.-W. 263 (1996) 581
Schneider, D.J., see Salikhov, K.M. 262 (1996) 17
Schneider, D.J., see Salikhov, K.M. 265 (1997) 562
Schneider, K.-P., Computer simulation of the surface roughness of lipid membranes 261 (1996) 81
Schneider, S., see Jäger, W. 270 (1997) 50
Schneider, W.F., see Hass, K.C. 263 (1996) 414
Schnieder, L., see Wrede, E. 265 (1997) 129
Schock, H.J., see Kim, J.U. 267 (1997) 323
Schoen, M. and D.J. Diestler, Liquid–vapor coexistence in a chemically heterogeneous slit-nanopore 270 (1997) 339
Scholes, G.D., D. Phillips and I.R. Gould, Low-lying excited states of 4-dimethylamino-benzonitrile: equilibrium geometries, vibrational frequencies and charge transfer character 266 (1997) 521
Schönnenbeck, G. and F. Stuhl, The HNCO + F reaction system: VUV-photolysis of the cyanato radical via Rydberg states 264 (1997) 199

Schoone, K., see Smets, J. 262 (1996) 789
Schreiber, E., see Heufelder, J. 269 (1997) 1
Schreiber, E., see Rutz, S. 269 (1997) 9
Schreiner, P.R., see Urban, J. 264 (1997) 441
Schriver, A., see Bahou, M. 265 (1997) 145
Schriver, A., see Moulin, V. 263 (1996) 423
Schriver-Mazzuoli, L., see Bahou, M. 265 (1997) 145
Schriver-Mazzuoli, L., see Moulin, V. 263 (1996) 423
Schulman, J.M. and R.L. Disch, Archimedene 262 (1996) 813
Schulte-Herbrüggen, T., see Mádi, Z.L. 268 (1997) 300
Schulz-Evers, M., see Teuchner, K. 268 (1997) 157
Schumm, S., M. Gerhards, W. Roth, H. Gier and K. Kleinermanns, A CASSCF study of the S_0 and S_1 states of phenol 263 (1996) 126
Schuppler, S., see Cummins, T.R. 261 (1996) 228
Schütz, M., see Schmidt, R. 263 (1996) 795
Schwartz, B.J., F. Hide, M.R. Andersson and A.J. Heeger, Ultrafast studies of stimulated emission and gain in solid films of conjugated polymers 265 (1997) 327
Schwarz, H., see Wörgötter, R. 270 (1997) 333
Schwegmann, S., A.P. Seitsonen, H. Dietrich, H. Bludau, H. Over, K. Jacobi and G. Ertl, The adsorption of atomic nitrogen on Ru(0001): geometry and energetics 264 (1997) 680
Schweiger, A., see Bingham, S.J. 266 (1997) 543
Schweiger, A., see Willer, M. 264 (1997) 1
Schweigert, V.A., see Alexandrov, A.L. 263 (1996) 551
Schweikhard, L., see Walther, C. 262 (1996) 668
Schweitzer, P., see Rübsam, M. 263 (1996) 540
Scott, G.B.I., D.A. Fairley, C.G. Freeman and M.J. McEwan, The reaction $H_3^+ + N$: a laboratory measurement 269 (1997) 88
Scuseria, G.E., see Maclagan, R.G.A.R. 262 (1996) 87
Scuseria, G.E., see Xu, C.H. 262 (1996) 219
Searle, B.G., see Harrison, N.M. 266 (1997) 507
Sebastian, K.L., see Chakravarti, N. 267 (1997) 9
Seddon, E.A., see Harrison, N.M. 266 (1997) 507
Seets, D.C., M.C. Wheeler and C.B. Mullins, Mechanism of the dissociative chemisorption of methane over Ir(110): trapping-mediated or direct? 266 (1997) 431
Seideman, T., see Haran, A. 268 (1997) 475
Seifert, G., P.W. Fowler, D. Mitchell, D. Porezag and Th. Frauenheim, Boron–nitrogen analogues of the fullerenes: electronic and structural properties 268 (1997) 352
Seinfeld, J.H., see Jungkamp, T.P.W. 263 (1996) 371
Seitsonen, A.P., see Schwegmann, S. 264 (1997) 680
Sekiguchi, S., K. Akiyama and S. Tero-Kubota, Positive exchange interaction in the radical ion pair of benzophenone anion and 1,4-diazabicyclo[2,2,2]octane cation radicals studied by FT-EPR spectroscopy 263 (1996) 161
Sekino, H., see Kirtman, B. 263 (1996) 313
Selloni, A., see Daul, C. 262 (1996) 74
Selzle, H.L., see Der Chao, S. 265 (1997) 445
Selzle, H.L., see Held, A. 267 (1997) 318
Semin, D.J., see Ambrose, W.P. 269 (1997) 365
Sen, R., A. Govindaraj and C.N.R. Rao, Carbon nanotubes by the metallocene route 267 (1997) 276

Senekowitsch, J., see Ramachandran, B. 270 (1997) 387
Senent, M.L., see Meléndez, F.J. 265 (1997) 649
Sengupta, A., M. Holtz and E.L. Quitevis, Temperature-dependent resonance Raman study of iodine-doped poly(vinyl alcohol) films 263 (1996) 25
Sengupta, D. and M.T. Nguyen, Ab initio calculations and quantum statistical analysis of the $SiH_3 + NO$ reaction 265 (1997) 35
Senn, G., B. Dünser, P. Scheier and T.D. Märk, Unimolecular dissociation of multiply-charged fullerene ions via the loss of intact C_6^+ units 266 (1997) 276
Senn, G., see Matejcik, S. 267 (1997) 329
Šepa, J., R.J. Gorte, D. White, E. Kassab and M. Allavena, The ^{13}C chemical shielding, ^{14}N quadrupole and the dipolar tensors of the nitrile group in the hydrogen-bonded acetonitrile–H-ZSM-5 adsorption complex 262 (1996) 321
Serrano, A. and S. Canuto, Quest for the ground state characterization of CaC 269 (1997) 193
Sesé, L.M., Quantum computation of the static structure factor of deuterium gas 266 (1997) 130
Setlik, B., see Andersen, J.N. 269 (1997) 371
Setser, D.W., see Butkovskaya, N.I. 266 (1997) 223
Setser, D.W., see Zikratov, G. 265 (1997) 585
Ševčík, P. and L. Adamčíková, Effect of a pressure decrease and stirring on the oscillating Bray–Liebhafsky reaction 267 (1997) 307
Sevian, A., M. Ravikanth and G.R. Kumar, Optical limiting in short chain basket handle porphyrins 263 (1996) 241
Shafigullin, M., see Alvarez, M.M. 266 (1997) 91
Shah, V., see Majumder, C. 261 (1996) 515
Shang, H., R. Gao, L. Ying, X. Zhao and Y. Tang, Laser induced dispersed fluorescence spectra of CH_3N radical and the lifetime of its $\tilde{A}^3E$ state 267 (1997) 345
Shank, C.V., see Cerullo, G. 262 (1996) 362
Shapira, Y., see Mishori, B. 264 (1997) 163
Sharma, R.D., see Duff, J.W. 265 (1997) 404
Shaw, A.M., see Carrington, A. 262 (1996) 598
Shen, H., P. Hvelplund, D.C. Lorents and D. Mathur, On the collisionally induced destruction of short- and long-lived fullerene ions 264 (1997) 508
Shen, L., see Zheng, G. 266 (1997) 533
Shen, Y., see Fang, J. 270 (1997) 145
Shen, Y.R., see Miranda, P.B. 264 (1997) 387
Shephard, M.J., see Bell, T.D.M. 268 (1997) 223
Shibamoto, Y., see Ueda, K. 261 (1996) 295
Shibata, T. and T. Suzuki, Photofragment ion imaging with femtosecond laser pulses 262 (1996) 115
Shigemoto, I., see Nakano, M. 262 (1996) 66
Shigemoto, I., see Yamada, S. 267 (1997) 438
Shigemoto, I., see Yamada, S. 267 (1997) 445
Shijun, Z., see Dianxun, W. 262 (1996) 776
Shimada, H., see Nibu, Y. 262 (1996) 615
Shimamori, H. and T. Sunagawa, Thermalization of electrons by collisions with CCl_4 in Ar buffer gas 267 (1997) 334
Shimizu, K., see Shimizu, S. 268 (1997) 93
Shimizu, S., M. Ikeguchi and K. Shimizu, Extracting contact free energy from solubility: excluded volume effects of polymers in continuum space 268 (1997) 93
Shin, S., see Ka, J. 269 (1997) 227

Shinohara, H., see Sugai, T. 264 (1997) 327
Shinohara, H., see Tomiyama, T. 264 (1997) 143
Shiotani, M., see Komaguchi, K. 265 (1997) 217
Shioya, T., see Bessho, K. 264 (1997) 381
Shirai, Y., see Abe, J. 261 (1996) 18
Shirakawa, M., see Imahori, H. 263 (1996) 545
Shirley, D.A., see Moler, E.J. 264 (1997) 502
Shirota, Y., see Nomura, S. 268 (1997) 461
Shizuka, H., see Yamaji, M. 261 (1996) 289
Shizuka, H., see Yoshihara, T. 261 (1996) 431
Shkrob, I.A., On the mechanism of multiplet CIDEP in radical ion pairs 264 (1997) 417
Shochat, S., see Spoyalov, A.P. 263 (1996) 715
Short, J., see Alexander, A.J. 262 (1996) 589
Shukla, A., M. Dolg, H. Stoll and P. Fulde, An ab initio embedded-cluster approach to electronic structure calculations on perfect solids: a Hartree–Fock study of lithium hydride 262 (1996) 213
Shushin, A.I., see Tarasov, V.V. 267 (1997) 58
Shuvalov, V.A., see Streltsov, A.M. 266 (1997) 347
Shvartsburg, A.A. and M.F. Jarrold, An exact hard-spheres scattering model for the mobilities of polyatomic ions 261 (1996) 86
Shvedko, A.G., see Kruglik, S.G. 270 (1997) 293
Si, J.-H., see Tian, H.-J. 263 (1996) 471
Sickafoose, S.M., P. Wikrent, B.J. Drouin and S.G. Kukolich, Microwave spectra and quadrupole coupling measurements for methyl rhenium trioxide 263 (1996) 191
Siebbeles, L.D.A. and Yu.A. Berlin, Diffusion in one-dimensional disordered systems: analytical study verified by Monte Carlo simulations 265 (1997) 460
Siebbeles, L.D.A., see Hilt, O. 269 (1997) 257
Siebert, S., see Müller, R. 262 (1996) 716
Siebrand, W., M.Z. Zgierski, Z.K. Smedarchina, M. Vener and J. Kaneti, The structure of phenol–ammonia clusters before and after proton transfer. A theoretical investigation 266 (1997) 47
Siehl, H.-U., see Stanton, J.F. 262 (1996) 183
Sievers, A.J., see Mungan, C.E. 270 (1997) 309
Silcocks, S.E., N. Jeffreys, F.M. Harris, S.R. Andrews and D.E. Parry, Double ionization of fluorobenzene to singlet and triplet states of its dication 262 (1996) 355
Sillesen, A., see Meunier, H. 261 (1996) 277
Sillman, P.D., see Mile, B. 263 (1996) 710
Silva, A.F., see Pereira, C.M. 268 (1997) 13
Silvente, E., R.C. Richter, M. Zheng, E.S. Saltzman and A.J. Hynes, Relative quantum yields for $O\,^1D$ production in the photolysis of ozone between 301 and 336 nm: evidence for the participation of a spin-forbidden channel 264 (1997) 309
Simons, J., see Boldyrev, A.I. 262 (1996) 807
Simons, J.P., see Alexander, A.J. 262 (1996) 589
Simpson, C.J.S.M., P.T. Griffiths, H.L. Wallaart and M. Towrie, Photodissociation of alkyl nitrites adsorbed on an MgF_2 surface. Rotational and translational energy distributions of product $NO(v, J)$ molecules 263 (1996) 19
Simpson, C.J.S.M., see Reid, J.P. 268 (1997) 150
Sinha, C., see Biswas, R. 263 (1996) 495
Sinha, C., see Biswas, R. 269 (1997) 186

Sinha, D., see Mitra, A. 261 (1996) 363
Sirotti, F., see Soriano, L. 266 (1997) 184
Skalny, J.D., see Matejcik, S. 261 (1996) 437
Skolnick, M.S., see Lidzey, D.G. 263 (1996) 655
Smalley, R.E., see Cowley, J.M. 265 (1997) 379
Smalley, R.E., see Nikolaev, P. 266 (1997) 422
Smart, B., C. Marsden, J.M. Hughes, F. Wang and E.I. von Nagy-Felsobuki, Variational calculations of the rovibrational energy levels of K_2Na^+ 261 (1996) 51
Smedarchina, Z.K., see Siebrand, W. 266 (1997) 47
Smelyansky, V.I. and J.S. Tse, The electronic structure of metallo-silicon clathrates Na_xSi_{136} ($x = 0$, 4, 8, 16 and 24) 264 (1997) 459
Smets, J., L. Houben, K. Schoone, G. Maes and L. Adamowicz, Multiple site proton affinities of methylated nucleic acid bases 262 (1996) 789
Smeyers, Y.G., see Meléndez, F.J. 265 (1997) 649
Smith, B.A., J.Z. Zhang, U. Giebel and G. Schmid, Direct probe of size-dependent electronic relaxation in single-sized Au and nearly monodisperse Pt colloidal nano-particles 270 (1997) 139
Smith, D.A., see Miaskiewicz, K. 270 (1997) 376
Smith, M.E., see Dirken, P.J. 266 (1997) 568
Smith, M.E., see Walters, J.K. 264 (1997) 539
Smith, T.A., see Bell, T.D.M. 268 (1997) 223
Smith, W., see Anderson, A. 263 (1996) 133
Smoluch, M., see Nowakowska, M. 270 (1997) 234
Snavely, D.L., see Grinevich, O. 267 (1997) 313
Snee, P.T., see Terzis, A.F. 264 (1997) 481
Snijders, J.G., see Biesheuvel, C.A. 269 (1997) 515
So, S.P., A Gaussian-2 molecular orbital study of the unimolecular reactions of acetyl cyanide 270 (1997) 363
Sobczyk, L., see Rospenk, M. 261 (1996) 283
Sobolewski, A.L., The cooperative dynamical Jahn–Teller effect in alkali doped fullerides 267 (1997) 452
Sodupe, M., see Baerends, E.J. 265 (1997) 481
Sokolov, N.D., see Vener, M.V. 264 (1997) 429
Sokolowski, M., see Gebauer, W. 266 (1997) 177
Sokołowski, S., see Trokhymchuk, A. 262 (1996) 33
Solca, J., see Huber, H. 266 (1997) 388
Solgadi, D., see Dedonder-Lardeux, C. 264 (1997) 596
Solís, J., see Castillejo, M. 268 (1997) 465
Somasundram, K., see Tozer, D.J. 265 (1997) 614
Song, M.-B., K. Yoshimi and M. Ito, STM observations of bridge-bonded CO on Pt(111) and asymmetric on-top CO on Pt(100) 263 (1996) 585
Song, N.W., T.-I. Kang, S.C. Jeoung, S.-J. Jeon, B.R. Cho and D. Kim, Improved method for measuring the first-order hyperpolarizability of organic NLO materials in solution by using the hyper-Rayleigh scattering technique 261 (1996) 307
Song, N.W., see Kim, Y. 264 (1997) 673
Soos, Z.G. and S.J. Schmidt, Equilibration with intrinsic traps in molecularly doped polymers 265 (1997) 427
Sorensen, S.L., see Andersen, J.N. 269 (1997) 371

Sorenson, J.M., J.K. Gregory and D.C. Clary, Diffusion Monte Carlo studies of isotope-substituted water trimers 263 (1996) 680
Soriano, L., M. Abbate, A. Fernández, A.R. González-Elipe, F. Sirotti, G. Rossi and J.M. Sanz, Thermal annealing of defects in highly defective NiO nanoparticles studied by X-ray and electron spectroscopies 266 (1997) 184
Soulard, P., see Asselin, P. 268 (1997) 265
Sousa, L.R., see Bhattacharyya, S. 269 (1997) 314
Sousa, M.J., see Pereira, C.M. 268 (1997) 13
Spackman, M.A. and P.G. Byrom, A novel definition of a molecule in a crystal 267 (1997) 215
Spano, F.C., see Antonova, S. 267 (1997) 158
Spath, B.W. and W.H. Miller, Semiclassical calculation of Franck–Condon intensities for reactive systems 262 (1996) 486
Spatola, P., see Laganà, A. 267 (1997) 403
Speiser, S., see Rosenblum, G. 263 (1996) 441
Spinelli, Yu., see Nizkorodov, S.A. 265 (1997) 303
Šponer, J. and P. Hobza, MP2 and CCSD(T) study on hydrogen bonding, aromatic stacking and nonaromatic stacking 267 (1997) 263
Šponer, J., see Hobza, P. 261 (1996) 379
Spoto, G., see Lamberti, C. 269 (1997) 500
Spoyalov, A.P., R.J. Hulsebosch, S. Shochat, P. Gast and A.J. Hoff, Evidence that Ala M260 is hydrogen-bonded to the reduced primary acceptor quinone $Q_A^{-\cdot}$ in reaction centers of *Rb. sphaeroides* 263 (1996) 715
Sreedhara Rao, V., see Chandra, A.K. 270 (1997) 87
St-Amant, A., see Goh, S.K. 264 (1997) 9
Stace, A.J., M.P. Dobson and C.A. Woodward, Metal complexes with unusual ligands: $Mg^+.(NO)_n$ 267 (1997) 171
Stamatovic, A., see Matejcik, S. 261 (1996) 437
Stangassinger, A., A.M. Knight and M.A. Duncan, Photoionization spectroscopy of NaAg 266 (1997) 189
Stankevich, I.V., see Gal'pern, E.G. 269 (1997) 85
Stanton, J.F., J. Gauss and H.-U. Siehl, CCSD(T) calculation of NMR chemical shifts: consistency of calculated and measured ^{13}C chemical shifts in the 1-cyclopropyl-cyclopropylidenemethyl cation 262 (1996) 183
Stanton, J.F., see Christiansen, O. 266 (1997) 53
Stanton, J.F., see Cui, Q. 263 (1996) 46
Stark, K., see Aoiz, F.J. 262 (1996) 175
Stark, K., see Aoiz, F.J. 264 (1997) 487
Staško, A., V. Brezová, P. Rapta, K.-D. Asmus and D.M. Guldi, [60]Fullerene anions in aqueous solutions (EPR study) 262 (1996) 233
Stavrev, K.K. and M.C. Zerner, Theoretical study of the Jahn–Teller effect on the spectroscopy of VCl_4 263 (1996) 667
Stec, W.J., see Uchimaru, T. 263 (1996) 691
Steer, R.P., see Abou-Zied, O.K. 266 (1997) 75
Steer, R.P., see Tittelbach-Helmrich, D. 262 (1996) 369
Stein, M. and J. Sauer, Formic acid tetramers: structure isomers in the gas phase 267 (1997) 111
Steinebrunner, G., see Huber, H. 266 (1997) 388
Stepanov, N.F., see Buchachenko, A.A. 261 (1996) 591
Stepanov, N.F., see Buchachenko, A.A. 269 (1997) 448
Stert, V., see Radloff, W. 261 (1996) 301

Stert, V., see Freudenberg, Th. 269 (1997) 523
Stert, V., see Radloff, W. 264 (1997) 210
Stevenson, S., see Grannan, S.M. 264 (1997) 359
Štich, I., see Miyazaki, T. 261 (1996) 346
Stimson, M.J., D.J. Ulness and A.C. Albrecht, Frequency and time resolved coherent Stokes Raman scattering in CS_2 using incoherent light 263 (1996) 185
Stoeckel, F., see Romanini, D. 270 (1997) 538
Stoeckel, F., see Romanini, D. 270 (1997) 546
Stoeckel, F., see Romanini, D. 264 (1997) 316
Stoeva, V., see Masoumi, Z. 261 (1996) 551
Stoll, H., see Shukla, A. 262 (1996) 213
Stolow, A., see Ivanov, M.Yu. 265 (1997) 231
Stolte, S., see Biesheuvel, C.A. 269 (1997) 515
Stolyarov, A.V., see Pazyuk, E.A. 267 (1997) 207
Stössel, R. and A.F. Münster, Experimental coupling of chemical oscillators by an excitable medium 263 (1996) 789
Straus, S.K., T. Bremi and R.R. Ernst, Resolution enhancement by homonuclear *J* decoupling in solid-state MAS NMR 262 (1996) 709
Strehlow, D., see Teuchner, K. 268 (1997) 157
Strek, W., see Deren, P.J. 264 (1997) 614
Streltsov, A.M., T.J. Aartsma, A.J. Hoff and V.A. Shuvalov, Oscillations within the B_L absorption band of *Rhodobacter sphaeroides* reaction centers upon 30 femtosecond excitation at 865 nm 266 (1997) 347
Struts, A.V., see Veracini, C.A. 263 (1996) 228
Stuchebrukhov, A.A., On the non-orthogonal basis set calculations of the bridge-mediated electronic matrix elements 265 (1997) 643
Stuhl, F., see Schönnenbeck, G. 264 (1997) 199
Su, M.-C., see Kumaran, S.S. 269 (1997) 99
Subramanian, V., K. Chitra, K. Venkatesh, S. Sanker and T. Ramasami, Comparative study on the vibrational IR spectra of cytosine and thiocytosine by various semi-empirical quantum mechanical methods 264 (1997) 92
Suenaga, Y., see Ueda, K. 261 (1996) 295
Sugai, I., see Yamazaki, T. 265 (1997) 137
Sugai, T. and H. Shinohara, Production and mass spectroscopic characterization of ammonium halide clusters 264 (1997) 327
Sugawara, K., see Nakanaga, T. 261 (1996) 414
Sugawara, K., see Nakanaga, T. 267 (1997) 491
Sugawara, K., see Trushin, S.A. 267 (1997) 573
Sugihara, G., see Oishi, O. 269 (1997) 530
Sugimoto, T., see Ueda, K. 261 (1996) 295
Suhai, S., see Mayer, I. 270 (1997) 211
Suhm, M.A., see Klopper, W. 261 (1996) 35
Suhm, M.A., see Quack, M. 269 (1997) 29
Sultan, R.F., The structural variety of chemical spike-electric field interactions 266 (1997) 145
Sumathi, R. and S.D. Peyerimhoff, A quantum statistical analysis of the rate constant for the $HO_2 + NH_2$ reaction 263 (1996) 742
Sun, C., see Ge, M. 264 (1997) 139
Sun, H., see Balasubramanian, K. 264 (1997) 70

Sun, W., see Ding, G. 265 (1997) 392
Sun, Y.-P., see Rollins, H.W. 268 (1997) 187
Sunagawa, T., see Shimamori, H. 267 (1997) 334
Sundholm, D., see Tokman, M. 265 (1997) 60
Sundström, V., see Chachisvilis, M. 261 (1996) 165
Suter, D., see Bingham, S.J. 266 (1997) 543
Suter, H.U. and B. Engels, An ab initio determination of the magnetic hyperfine structure of C_2 in the four lowest triplet states 261 (1996) 644
Sutjianto, A. and L.A. Curtiss, Theoretical study of the potential energy surface of diglyme 264 (1997) 127
Suto, K., see Yamaji, M. 261 (1996) 289
Suvernev, A.A. and D.Z. Goodson, Dimensional perturbation theory: an efficient method for computing vibration–rotation spectra 269 (1997) 177
Suvernev, A.A., see Tadday, R. 268 (1997) 117
Suwaiyan, A., see Than Htun, M. 264 (1997) 285
Suzuki, S., see Qin, L.-C. 268 (1997) 101
Suzuki, T., T. Ichimura, M. Kusaba and N. Nakashima, Reaction dynamics of hot naphthalene molecules in the gas phase with ArF laser excitation 263 (1996) 197
Suzuki, T., U. Okuyama and T. Ichimura, Direct determination of reaction heat in intramolecular hydrogen abstraction of excited 2-methylbenzophenone 266 (1997) 107
Suzuki, T., see Shibata, T. 262 (1996) 115
Suzuki, T., see Hashimoto, N. 264 (1997) 545
Suzuki, Y., S. Asai, K. Kobayashi, T. Noro, F. Sasaki and H. Tatewaki, Potential curves of the ground state and low-lying states of the scandium dimer using state-averaged MCSCF orbitals 268 (1997) 213
Svanberg, M. and J.B.C. Pettersson, Survival of noble gas clusters scattering from hot metal surfaces 263 (1996) 661
Swarnabala, G., M.V. Rajasekharan and S. Padhye, Origin of the hyperfine anisotropy in a Mn(IV) complex containing paramagnetic ligands 267 (1997) 539
Sworakowski, J., see Mergulhão, S. 269 (1997) 489
Symons, M.C.R., see Mishra, S.P. 263 (1996) 476
Syrrou, M., see Georgiou, S. 270 (1997) 491
Szablewski, M., see Cross, G.H. 268 (1997) 36
Szajdzinska-Pietek, E. and M. Wolszczak, Quenching of pyrene fluorescence by amphiphilic nitroxide radicals embedded in cationic micelles 270 (1997) 527
Szalay, P.G. and G. Fogarasi, Theoretical prediction of the electronic excited states and resonance Raman intensities in formamide from coupled cluster calculations 270 (1997) 406
Szalay, P.G., G. Fogarasi and L. Nemes, Quantum chemical coupled cluster study of the structure and spectra of the ground and first excited states of the ketenyl radical 263 (1996) 91
Szalewicz, K., see Williams, H.L. 262 (1996) 431
Szczepaniak, K., see Del Bene, J.E. 264 (1997) 109
Szwarc, H., see Agafonov, V. 267 (1997) 193

Taatjes, C.A., see Thiesemann, H. 270 (1997) 580
Tachikawa, H., Electronic structures of linear polysilane radical cations ground and low-lying excited states: a theoretical study 265 (1997) 455
Tadday, R., A.A. Suvernev, T. Dreier and J. Wolfrum, Quantum beat spectroscopy of OH radicals in atmospheric pressure flames 268 (1997) 117
Taferner, W.T. and S.G. Davison, Chemisorption on substrates with long-range interactions 269 (1997) 171

Tahara, T., see Matsuo, S. 264 (1997) 636
Taira, K., see Uchimaru, T. 263 (1996) 691
Takada, T., see Tomonari, M. 266 (1997) 488
Takahashi, H., T. Kasai and K. Yamaguchi, Wavepacket dynamics in the full reaction of $CF_3H + Ar(^3P) \rightarrow CF_3^* + H + Ar$: quantum interference for the H-end orientation 264 (1997) 44
Takahashi, K. and C.D. Jonah, The measurement of an electron transfer reaction in a non-polar supercritical fluid 264 (1997) 297
Takami, M., see Geng, J. 266 (1997) 290
Takami, M., see Jakubek, Z.J. 265 (1997) 653
Takayanagi, T. and G.C. Schatz, Quantum reactive scattering studies of the $CN + H_2 \rightarrow HCN + H$ reaction: the role of the non-reactive CN bond 265 (1997) 410
Takeda, K., see Mitsui, M. 262 (1996) 125
Takeda, S., see Kawakami, T. 261 (1996) 129
Takeo, H., see Nakanaga, T. 261 (1996) 414
Takeo, H., see Trushin, S.A. 267 (1997) 573
Takeshima, M. and A.H. Matsui, Frenkel exciton states in microcrystallites 266 (1997) 135
Talbi, D. and Y. Ellinger, Isomerization versus hydrogen exchange reaction in the HNC ⇌ HCN conversion 263 (1996) 385
Talukdar, R.K., M. Hunter, R.F. Warren, J.B. Burkholder and A.R. Ravishankara, UV laser photodissociation of CF_2ClBr and CF_2Br_2 at 298 K: quantum yields of Cl, Br, and CF_2 262 (1996) 669
Talukdar, R.K., see Rudich, Y. 261 (1996) 467
Tamai, N., see Miyasaka, H. 269 (1997) 281
Tamura, H., see Yamazaki, T. 265 (1997) 137
Tanabe, K., see Uchimaru, T. 263 (1996) 691
Tanabe, K., see Uchimaru, T. 267 (1997) 244
Tanaka, K., see Ishiguro, M. 263 (1996) 629
Tanaka, K., see Matsuzaki, Y. 263 (1996) 119
Tanaka, M., see Tsuji, M. 262 (1996) 349
Tanaka, M., see Tsuji, M. 266 (1997) 246
Tanaka, T., see Ishiguro, M. 263 (1996) 629
Tanaka, T., see Yamaji, M. 261 (1996) 289
Tanarro, I., see Aoiz, F.J. 262 (1996) 175
Tang, A.C. and F.Q. Huang, Electronic structures of octahedral fullerenes 263 (1996) 733
Tang, H. and D.H. Zhang, Studies on determination of degree of coupling of Fermi resonance 265 (1997) 84
Tang, H.R., see Wang, Y.L. 268 (1997) 387
Tang, Y., see Shang, H. 267 (1997) 345
Taniguchi, S., see Imahori, H. 263 (1996) 545
Tanimoto, Y., see Harima, Y. 267 (1997) 481
Tanimura, K., see Itoh, C. 261 (1996) 191
Tanimura, Y., see Tomita, N. 263 (1996) 687
Tannor, D., see Garashchuk, S. 262 (1996) 477
Tannor, D.J., see Garashchuk, S. 263 (1996) 324
Tapia, O., see Pérez, P. 269 (1997) 419
Tarasov, V.V., G.E. Zoriniants, A.I. Shushin and M.M. Triebel, The role of spin–lattice relaxation in magnetic field effects on the luminescence of amorphous and polycrystalline rubrene films 267 (1997) 58
Tarrach, G., see Bopp, M.A. 263 (1996) 721

Tassaing, T., M. Besnard and J. Yarwood, Far IR vibrational spectroscopic studies of the chemical dynamics of the pyridine/iodine system in solution 267 (1997) 496
Tasumi, M., see Hirata, S. 261 (1996) 241
Tatewaki, H., see Suzuki, Y. 268 (1997) 213
Taylor, S.M., see Carrington, A. 262 (1996) 598
Teki, Y., K. Itoh, A. Okada, H. Yamakage, T. Kobayashi, K. Amaya, S. Kurokawa, S. Ueno and Y. Miura, Magnetic properties of stable N-[(dichlorophenyl)thio]-2,4,6-triphenylphenylaminyl and N-[(dichlorophenyl)thio]-2,4,6-tris(chlorophenyl)phenylaminyl radical crystals 270 (1997) 573
Telnov, D.A. and S.-I Chu, Floquet formulation of time-dependent density functional theory 264 (1997) 466
Temsamani, M.A. and H. Herman, Anharmonic resonances in monodeuteroacetylene ($^{12}C_2HD$) (Chem. Phys. Letters 260 (1996) 253). Erratum 264 (1997) 556
Ten-no, S., see Tomita, N. 263 (1996) 687
ten Grotenhuis, E., J.C. van Miltenburg and J.P. van der Eerden, Preparation of anthracene micro-crystals by spin-coating and atomic force microscopy study of the molecular packing 261 (1996) 558
Terakura, K., see Miyazaki, T. 261 (1996) 346
Teramae, H., see Imhof, R. 270 (1997) 500
Teramae, N., see Bessho, K. 264 (1997) 381
Terasaki, A., H. Yamaguchi, H. Yasumatsu and T. Kondow, Fragmentation dynamics of silicon cluster anions in collision with a silicon surface: contrast to aluminum cluster anions 262 (1996) 269
Terblanche, C.J., see Reynhardt, E.C. 269 (1997) 464
ter Meulen, J.J., see Drabbels, M. 267 (1997) 127
ter Meulen, J.J., see Marijnissen, A. 263 (1996) 803
Tero-Kubota, S., see Sekiguchi, S. 263 (1996) 161
Terrones, H., see Hsu, W.K. 262 (1996) 161
Terrones, M., see Hsu, W.K. 262 (1996) 161
ter Steege, D.H.A., see Biesheuvel, C.A. 269 (1997) 515
Terzis, A.F., P.T. Snee and E.T. Samulski, Orientational order of water confined in anisotropic cavities 264 (1997) 481
Teuchner, K., M. Schulz-Evers, D. Leupold, D. Strehlow and W. Rüdiger, The complex excited state dynamics of the early photocycle of phytochrome 268 (1997) 157
Thaddeus, P., see McCarthy, M.C. 264 (1997) 252
Thakkar, A.J., see Bündgen, P. 261 (1996) 625
Than Htun, M., A. Suwaiyan and U.K.A. Klein, Effects of calcium chloride on the proton transfer dynamics of 4-hydroxy-1-naphthalenesulphonate in alcohol/water mixtures 264 (1997) 285
Thess, A., see Cowley, J.M. 265 (1997) 379
Thess, A., see Nikolaev, P. 266 (1997) 422
Thevuthasan, S., see Chambers, S.A. 267 (1997) 51
Thibault, F., see Khalil, B. 263 (1996) 811
Thiel, W., see Breidung, J. 266 (1997) 515
Thienpont, H., see Verbandt, Y. 270 (1997) 471
Thiesemann, H. and C.A. Taatjes, Temperature dependence of the reaction C_2H (C_2D) + O_2 between 295 and 700 K 270 (1997) 580
Thomson, A.J., see Bingham, S.J. 266 (1997) 543

Tian, H.-J., H.-F. Mao, Q.-F. Zhou, H.-J. Xu, J.-H. Si, Y. Wang, Q. Yang and P.-X. Ye, Photoinduced electron transfer and dynamic behavior of charge-separated state nonlinear optical process in a self-assembled porphyrin supramolecular system 263 (1996) 471
Tian, Z.Q., see Gao, J.S. 262 (1996) 151
Tikhov, M.S., see Lomas, J.R. 263 (1996) 591
Tilquin, J.-Y., see Gilliams, B. 269 (1997) 509
Tilwankar, S., see Agrawal, P.M. 266 (1997) 481
Tittelbach-Helmrich, D. and R.P. Steer, Subpicosecond population decay time of the first excited singlet state of thioxanthione in fluid solution 262 (1996) 369
Tiwary, D., see Mishra, S.P. 263 (1996) 476
Tkachenko, N.V., P.H. Hynninen and H. Lemmetyinen, Photoelectric signals of chlorophyll *a* Langmuir–Blodgett films 261 (1996) 234
Tober, E., see Chambers, S.A. 267 (1997) 51
Tobiason, J.D. and E.A. Rohlfing, Reply to the Comment on "Lifetimes of vibrational levels in the $\tilde{B}\ ^2A'$ state of HCO" 261 (1996) 387
Tokeshi, M., K. Nakashima and T. Ogawa, Direct collisional scattering of the excited hydrogen atom: Doppler profile analysis in fast Ar^+ ion collisions with acetylene and ethylene 263 (1996) 783
Tokman, M., D. Sundholm, P. Pyykkö and J. Olsen, The nuclear quadrupole moment of ^{14}N obtained from finite-element MCHF calculations on N^{2+} ($2p;\ ^2P_{3/2}$) and N^+ ($2p^2;\ ^3P_2$ and $2p^2;\ ^1D_2$) 265 (1997) 60
Tokue, I., T. Kawai and K. Yamasaki, Rotational excitation of ions produced by the He($2\ ^3S$) Penning ionization of CO and N_2 270 (1997) 587
Tokumoto, M., see Nakashima, S. 268 (1997) 359
Tokunaga, F., see Chosrowjan, H. 270 (1997) 267
Tománek, D., see Lee, Y.H. 265 (1997) 667
Tománek, D., see Grönbeck, H. 264 (1997) 39
Tománek, D., see Kim, S.G. 264 (1997) 345
Tominaga, K., see Saitow, K. 262 (1996) 621
Tomita, N., S. Ten-no and Y. Tanimura, Ab initio molecular orbital calculations by the resonating Hartree–Fock approach: superposition of non-orthogonal Slater determinants 263 (1996) 687
Tomiyama, T., S. Uchiyama and H. Shinohara, Solubility and partial specific volumes of C_{60} and C_{70} 264 (1997) 143
Tomkinson, J., see Hirata, S. 261 (1996) 241
Tomonari, M., N. Ookubo and T. Takada, Molecular hyperpolarizability components β_{zzz} and β_{zxx} under directional extensions of π conjugation: missing-orbital analysis and simplified sum-over-states calculations 266 (1997) 488
Topp, M.R., see Andrews, P.M. 265 (1997) 224
Topp, M.R., see Pryor, B.A. 267 (1997) 531
Torii, H., see Hirata, S. 261 (1996) 241
Torii, H.A., see Yamazaki, T. 265 (1997) 137
Tortajada, J., see Luna, A. 266 (1997) 31
Tóth, G., The structure of dilute polymer colloid suspensions as seen by the reverse Monte Carlo method 269 (1997) 413
Toth, L.M., see Dai, S. 262 (1996) 315
Towrie, M., see Simpson, C.J.S.M. 263 (1996) 19
Toyota, N., see Ueda, K. 261 (1996) 295

Tozer, D.J., K. Somasundram and N.C. Handy, On the accuracy of molecular exchange–correlation potentials computed from electron densities 265 (1997) 614
Trajmar, S. and I. Kanik, Electron impact excitation of C_{60} adducts; fluorescence from $C_{60}OH$ and $C_{60}H$ species 262 (1996) 241
Travers, M.J., see McCarthy, M.C. 264 (1997) 252
Treindl, L., T. Hemmingsen and P. Ruoff, Belousov–Zhabotinsky oscillations during the chemical or electrochemical generation of Ag^+ ions 269 (1997) 263
Treindl, L., see Olexová, A. 268 (1997) 505
Tretyakov, Yu.D., see Vertegel, A.A. 262 (1996) 455
Treutler, O., see Bauernschmitt, R. 264 (1996) 573
Triebel, M.M., see Frankevich, E.L. 261 (1996) 545
Triebel, M.M., see Tarasov, V.V. 267 (1997) 58
Trifunac, A.D., see Werst, D.W. 269 (1997) 333
Tritt-Goc, J., N. Piślewski and S.K. Hoffmann, EPR evidence of the paramagnetism of a long-living metastable excited state of a sodium nitroprusside single crystal 268 (1997) 471
Trokhymchuk, A., O. Pizio, D. Henderson and S. Sokołowski, The reference inhomogeneous Percus–Yevick approximation for a dimerizing fluid near a hard wall 262 (1996) 33
Tronc, M., see Hedhili, M.N. 268 (1997) 21
Troxler, T., see Xue, B. 265 (1997) 154
Trunk, M., J. Popp, M. Lankers and W. Kiefer, Microchemistry: time dependence of an acid-base reaction in a single optically levitated microdroplet 264 (1997) 233
Trushin, S., see Fuß, W. 262 (1996) 675
Trushin, S.A., K. Sugawara and H. Takeo, Observation of CrCO in the 5 μm multiphoton decomposition of $Cr(CO)_6$ 267 (1997) 573
Tsaune, A.Ya., see Glushkov, V.N. 262 (1996) 59
Tse, J.S., see Smelyansky, V.I. 264 (1997) 459
Tse, T.Y., see Vold, R.L. 263 (1996) 271
Tserepi, A.D., E. Wurzberg and T.A. Miller, Two-photon-excited stimulated emission from atomic oxygen in rf plasmas: detection and estimation of its threshold 265 (1997) 297
Tsuchida, A., see Ohkita, H. 263 (1996) 602
Tsuji, M., M. Tanaka and Y. Nishimura, New emission spectra of $KrXe^+$ produced from Kr afterglow reactions of Xe 262 (1996) 349
Tsuji, M., M. Tanaka and Y. Nishimura, The $B\,1/2 \rightarrow X\,1/2$ and $C_2\,1/2 \rightarrow A_2\,1/2$ transitions of $ArKr^+$ produced from argon afterglow reactions of Kr 266 (1997) 246
Tsukuda, T., M.A. Johnson and T. Nagata, Photoelectron spectroscopy of $(CO_2)_n^-$ revisited: core switching in the $2 \leqslant n \leqslant 16$ range 268 (1997) 429
Tsukuda, T., T. Kondow, C.E.H. Dessent, C.G. Bailey, M.A. Johnson, J.H. Hendricks, S.A. Lyapustina and K.H. Bowen, Characterization of the anionic intracluster polymerization reaction product of 2-chloroacrylonitrile trimers by photoelectron spectroscopy 269 (1997) 17
Tsumura, T., see Maeyama, T. 264 (1997) 292
Tsuneda, T. and K. Hirao, A new spin-polarized Colle–Salvetti-type correlation energy functional 268 (1997) 510
Tsuzuki, S., see Uchimaru, T. 263 (1996) 691
Tsvetkov, Yu.D., see Dzuba, S.A. 264 (1997) 238
Tuckett, R.P. and P.J. Knowles, The geometry of the $\tilde{X}\,^2A_1$ state of PF_3^+: experiment and theory 261 (1996) 486
Tunega, D., J. Noga and W. Klopper, Basis set limit value for the static dipole polarizability of beryllium 269 (1997) 435

Tureček, F., see Sadílek, M. 263 (1996) 203
Turnes Palomino, G., see Lamberti, C. 269 (1997) 500
Turpin, P.-Y., see Kruglik, S.G. 270 (1997) 293
Turton, S., see Jones, R.G. 261 (1996) 539
Tzannis, A.P., see Radi, P.P. 265 (1997) 271

Ubachs, W., Predissociative decay of the $c_4'\,^1\Sigma_u^+$, $v = 0$ state of N_2 268 (1997) 201
Uchida, T., see Bessho, K. 264 (1997) 381
Uchimaru, T., R. Hara, K. Tanabe and K. Fujimori, Acyloxyl radical pair intermediate for the initial stage of the thermal decomposition of diacyl peroxide: a density functional study 267 (1997) 244
Uchimaru, T., W.J. Stec, S. Tsuzuki, T. Hirose, K. Tanabe and K. Taira, Ab initio investigation on nucleophilic ring opening of 1,3,2-oxathiaphospholane: nucleophilic substitution at phosphorus coupled with pseudorotation 263 (1996) 691
Uchiyama, S., see Tomiyama, T. 264 (1997) 143
Uda, T., see Miyazaki, T. 261 (1996) 346
Ueda, K., T. Sugimoto, S. Endo, N. Toyota, M. Kohama, K. Yamamoto, Y. Suenaga, H. Morimoto, T. Yamaguchi, M. Munakata, N. Hosoito, N. Kanehisa, Y. Shibamoto and Y. Kai, 1:2 TCNQ/$TCNQ^{-\cdot}$ mixed salts exhibiting ferromagnetic behavior at room temperature 261 (1996) 295
Ueda, M., see Kamada, K. 263 (1996) 215
Ueda, M., see Kamada, K. 267 (1997) 402
Ueno, S., see Teki, Y. 270 (1997) 573
Ulenikov, O.N., S. Alanko, M. Koivusaari and R. Anttila, Ground state ''supercombination differences'' as the method of determination of splittings for faintly polar symmetric top molecules: the CHD_3 molecule 268 (1997) 242
Ulic, S.E., see Gobbato, K.I. 266 (1997) 527
Ullmann, G., see Volke, F. 262 (1996) 374
Ulness, D.J., see Stimson, M.J. 263 (1996) 185
Umapathy, S., see Balakrishnan, G. 270 (1997) 557
Umbach, E., see Gebauer, W. 266 (1997) 177
Umemoto, H., Y. Kimura and T. Asai, Production of $NH(X^3\Sigma^-)$ radicals in the reaction of $N(2^2D)$ with CH_4: nascent rotational and vibrational distributions of NH 264 (1997) 215
Urban, J., P.R. Schreiner, G. Vacek, P. von R. Schleyer, J.Q. Huang and J. Leszczynski, Molecular structures, vibrational spectra and rotational barriers of C_2H_6, Si_2H_6, $SiGeH_6$ and Ge_2H_6 – experiment and theory in harmony 264 (1997) 441
Urbanski, K., see Antonova, S. 267 (1997) 158
Usaj, G., see Pastawski, H.M. 261 (1996) 329

Vaara, J., see Koskela, T. 261 (1996) 425
Vaara, J., see Hyvönen, M. 268 (1997) 55
Vaccaro, P.H., see Müller, T. 266 (1997) 575
Vaccaro, P.H., see Wasserman, T.A.W. 262 (1996) 329
Vacek, G., see Urban, J. 264 (1997) 441
Vaksman, M.A., The study of anisotropy of gas–surface scattering using surface light-induced drift 267 (1997) 77
Valbusa, U., see Buatier de Mongeot, F. 270 (1997) 345
Valeur, B., see Fedorov, A. 267 (1997) 467

Van Amerongen, H., see Peterman, E.J.G. 264 (1997) 279
Van Brederode, M.E., M.R. Jones and R. Van Grondelle, Fluorescence excitation spectra of membrane-bound photosynthetic reaction centers of *Rhodobacter sphaeroides* in which the tyrosine M210 residue is replaced by tryptophan: evidence for a new pathway of charge separation 268 (1997) 143
Van Campen, D.G., see Hrbek, J. 267 (1997) 65
Van Dam, L., B. Andreasson and L. Nordenskiöld, Multiple-quantum pulsed gradient NMR diffusion experiments on quadrupolar ($I > 1/2$) spins 262 (1996) 737
Van den Berg, E., see Engeln, R. 269 (1997) 293
Van der Auweraer, M., see Imans, F. 262 (1996) 583
Van der Auweraer, M., see Scheblykin, I.G. 261 (1996) 181
Van der Auweraer, M., see Argyrakis, P. 268 (1997) 372
Van der Auweraer, M., see Chattopadhyay, N. 264 (1997) 265
Van der Avoird, A., see Moszynski, R. 263 (1996) 107
Van der Eerden, J.P., see ten Grotenhuis, E. 261 (1996) 558
Van der Klink, J.J., see Vuissoz, P.-A. 264 (1997) 366
Van der Meer, A.F.G., see Maas, D.J. 270 (1997) 45
Van der Meer, A.F.G., see Engeln, R. 269 (1997) 293
Van der Veldt, T., see Berden, G. 265 (1997) 204
Van der Zande, W.J., see Maas, D.J. 270 (1997) 45
Van Dijken, A., D. Vanmaekelbergh and A. Meijerink, Size selective photoetching of nanocrystalline CdS particles 269 (1997) 494
Van Eck, E.R.H., see Dirken, P.J. 266 (1997) 568
Van Es, S., see Hendrickx, E. 270 (1997) 241
Van Essenberg, W., see Jenniskens, H.G. 268 (1997) 7
Van Grondelle, R., see Van Brederode, M.E. 268 (1997) 143
Van Grondelle, R., see Baltuška, A. 270 (1997) 263
Van Grondelle, R., see Peterman, E.J.G. 264 (1997) 279
Van Herck, K., see Binnemans, K. 266 (1997) 297
Van Hoek, A., see Fisz, J.J. 270 (1997) 432
Van Look, H., see Devriendt, K. 261 (1996) 450
Van Loosdrecht, P.H.M., see Grannan, S.M. 264 (1997) 359
Vanmaekelbergh, D., see van Dijken, A. 269 (1997) 494
Van Miltenburg, J.C., see ten Grotenhuis, E. 261 (1996) 558
Van Orden, A., see Enderlein, J. 270 (1997) 464
Van Stokkum, I.H.M., see Baltuška, A. 270 (1997) 263
Van Stokkum, I.H.M., see Peterman, E.J.G. 264 (1997) 279
Van Stryland, E.W., see Díaz-García, M.A. 266 (1997) 86
Van Zee, R.J. and W. Weltner Jr., Quenching of the orbitally-degenerate nickel, palladium, and platinum cations (d^9, $^2D_{5/2}$) in rare-gas matrices: ESR evidence 266 (1997) 403
Van Zee, R.J., see Li, S. 262 (1996) 298
Varnavsky, O.P., see Scheblykin, I.G. 261 (1996) 181
Varnavsky, O.P., see Argyrakis, P. 268 (1997) 372
Vasiliev, G.K., see Aleinikov, N.N. 267 (1997) 155
Vatsa, R.K., see Brownsword, R.A. 266 (1997) 259
Veciana, J., see Deumal, M. 265 (1997) 190
Vecli, A., see Bonetti, G. 269 (1997) 268
Vela, A., see Pérez, P. 269 (1997) 419

Velasco, A.M., I. Martin and C. Lavín, Rydberg electron transitions in the methyl radical 264 (1997) 579
Velegrakis, M., see Lüder, C. 267 (1997) 149
Velic, D. and R.J. Levis, A model for estimating the surface effective mass during collision-induced processes on Pt{111} 269 (1997) 59
Vener, M., see Siebrand, W. 266 (1997) 47
Vener, M.V. and N.D. Sokolov, On the adiabatic separation of the vibrational variables of a hydrogen-bonded AHA fragment with a symmetric double-well potential 264 (1997) 429
Venkatesh, K., see Subramanian, V. 264 (1997) 92
Veracini, C.A., A.V. Struts and O.F. Bezrukov, The study of water diffusion in the lamellar phase of water–ammonium perfluorononanoate mixture 263 (1996) 228
Verbandt, Y., H. Thienpont, I. Veretennicoff, P. Geerlings and G.L.J.A. Rikken, Origin of the saturation of the third-order optical nonlinear response of one-dimensional conjugated systems 270 (1997) 471
Verel, R., see Verhoeven, A. 266 (1997) 465
Veretennicoff, I., see Verbandt, Y. 270 (1997) 471
Verhoeven, A., R. Verel and B.H. Meier, J cross polarization in magic-angle-spinning NMR 266 (1997) 465
Verhoeven, J.W., see Jäger, W. 270 (1997) 50
Verhoeven, J.W., see Middelhoek, E.R. 267 (1997) 525
Verma, A.L., S. Sato and T. Kitagawa, Time-resolved resonance Raman evidence for the exciplex formation of free-base porphyrin with an electron acceptor 267 (1997) 507
Vertegel, A.A., S.V. Kalinin, N.N. Oleynikov and Yu.D. Tretyakov, Visible spectra of fractal particles in colloidal solutions 262 (1996) 455
Vervloet, M., see Hadj Bachir, I. 270 (1997) 533
Vezmar, I., see Alvarez, M.M. 266 (1997) 91
Viaene, L., see Imans, F. 262 (1996) 583
Viappiani, C., see Bonetti, G. 269 (1997) 268
Videira, A.L.L., see Carlos, L.D. 264 (1997) 57
Vieth, H.-M., see Dvinskikh, S.V. 268 (1997) 401
Vigasin, A.A., see Huisken, F. 269 (1997) 235
Vijayalakshmi, K., C.P. Safvan, G. Ravindra Kumar and D. Mathur, On the ionization and dissociation of NO_2 by short intense laser pulses 270 (1997) 37
Villarreal, P., see Buchachenko, A.A. 269 (1997) 448
Viruela, P.M., see Sastre, G. 264 (1997) 565
Visschers, R.W., see Kumble, R. 261 (1996) 396
Vitukhnovsky, A.G., see Scheblykin, I.G. 261 (1996) 181
Vitukhnovsky, A.G., see Argyrakis, P. 268 (1997) 372
Vogel, H.-P., see Helm, R.M. 270 (1997) 285
Vohs, J.M., see Plank, R.V. 263 (1996) 33
Vold, R.L., G.L. Hoatson and T.Y. Tse, Effects of slow motion on deuteron relaxation time anisotropy 263 (1996) 271
Volke, F., A. Pampel, M. Haensler and G. Ullmann, Proton MAS NMR of a protein in a frozen aqueous solution 262 (1996) 374
Volkmer, A., D.A. Hatrick, Y. Bai and D.J.S. Birch, Femtosecond three-photon excitation and single-photon timing detection of α-NPO fluorescence 268 (1997) 439
Volpp, H.-R., see Brownsword, R.A. 266 (1997) 259
Von Borczyskowski, C., see Wrachtrup, J. 267 (1997) 179
Vondrák, T., S. Sato and K. Kimura, Zero kinetic energy photoelectron study of the naphthalene–Ar van der Waals complex 261 (1996) 481

Von Egidy, T., see Yamazaki, T. 265 (1997) 137
Von Helden, G., see Engeln, R. 262 (1996) 105
Von Helden, G., see Jongma, R.T. 270 (1997) 304
Von Nagy-Felsobuki, E.I., see Smart, B. 261 (1996) 51
Von Nagy-Felsobuki, E.I., see Wang, F. 269 (1997) 138
Vörtler, H.L. and M. Kettler, Monte Carlo simulation of pore systems: primitive model of water in slit-like pores 266 (1997) 368
Voth, G.A., see Calhoun, A. 262 (1996) 415
Voth, G.A., see Cao, J. 261 (1996) 111
Vourliotaki, A., see Lüder, C. 267 (1997) 149
Vuissoz, P.-A., T. Yonezawa, D. Yang, J. Kiwi and J.J. van der Klink, ^{103}Rh NMR in small rhodium particles 264 (1997) 366

Wada, A., see Fujino, T. 261 (1996) 534
Waga, M., S. Maki, F. Hashimoto and H. Sakuragi, Excitation wavelength dependence of the Z → E one-way isomerization of 4-halostilbene radical cations in excited states 265 (1997) 277
Wakabayashi, F., see Fujino, T. 261 (1996) 534
Waldfried, C., see McIlroy, D.N. 264 (1997) 168
Wales, D.J., see Doye, J.P.K. 262 (1996) 167
Wales, D.J., see Doye, J.P.K. 269 (1997) 408
Wall, T., see Gadd, G.E. 270 (1997) 108
Wallaart, H.L., see Simpson, C.J.S.M. 263 (1996) 19
Wallace, S.C., see Abou-Zied, O.K. 266 (1997) 75
Walser, D., T. Plakhotnik, A. Renn and U.P. Wild, One- and two-photon spectroscopy on single molecules of diphenyloctatetraene 270 (1997) 16
Walser, D., see Plakhotnik, T. 262 (1996) 379
Walters, J.K., J.S. Rigden, P.J. Dirken, M.E. Smith, W.S. Howells and R.J. Newport, An atomic-scale study of the role of titanium in TiO_2:SiO_2 sol–gel materials 264 (1997) 539
Walther, C., G. Dietrich, M. Lindinger, K. Lützenkirchen, L. Schweikhard and J. Ziegler, Time resolved photofragmentation of Au_{15}^+ clusters (Chem. Phys. Lett. 256 (1996) 77). Erratum 262 (1996) 668
Walton, D.R.M., see Hsu, W.K. 262 (1996) 161
Wandel, H., see Kraka, E. 268 (1997) 313
Wang, C.-R., K.K.-W. Lo and V.W.-W. Yam, Ab initio study of luminescent chalcogenido silver(I) clusters $[Ag_4(\mu\text{-}H_2PCH_2PH_2)_4(\mu_4\text{-}E)]^{2+}$ 262 (1996) 91
Wang, D., X. Qian and Q. Zhang, The isonitrile–nitrile isomerization: kinetic parameters, reaction mechanism and relative photoionization cross-section of the HOMO. A HeI photoelectron spectroscopy study 266 (1997) 560
Wang, E.G., see Guo, L.P. 268 (1997) 26
Wang, F., F.R.W. McCourt and E.I. von Nagy-Felsobuki, Ab initio potential energy surface and vibrational energies of Li_3^- 269 (1997) 138
Wang, F., see Smart, B. 261 (1996) 51
Wang, J., see Zhu, T. 265 (1997) 334
Wang, J., see Holmlid, L. 268 (1997) 285
Wang, L. and D.C. Clary, A quenching method in quantum–classical studies of dynamics with a bifurcating wavefunction 262 (1996) 284
Wang, Q., see Cerullo, G. 262 (1996) 362
Wang, S.-L. and T.-I. Ho, Protonation dependent electron transfer in 2-styrylquinolines 268 (1997) 434

Wang, W., M.J. Feldstein and N.F. Scherer, Observation of coherent multiple scattering of surface plasmon polaritons on Ag and Au surfaces 262 (1996) 573
Wang, W.N., see Huang, H.H. 265 (1997) 508
Wang, X., see Li, L. 262 (1996) 52
Wang, X., see Li, L. 268 (1997) 549
Wang, Y., see Feng, W.L. 266 (1997) 43
Wang, Y., see Tian, H.-J. 263 (1996) 471
Wang, Y.A., S. Liu and R.G. Parr, Laurent series expansions in density functional theory 267 (1997) 14
Wang, Y.A., Padé approximants in density functional theory 268 (1997) 76
Wang, Y.L., P.S. Belton and H.R. Tang, Proton NMR relaxation studies of solid L-alaninamide 268 (1997) 387
Wang, Y.Q., see Zhu, T. 265 (1997) 334
Wang, Z., see Chambers, S.A. 267 (1997) 51
Wang, Z., see Han, J. 265 (1997) 209
Wängberg, I., I. Barnes and K.H. Becker, Atmospheric chemistry of bifunctional cycloalkyl nitrates 261 (1996) 138
Warman, J.M., see Gelinck, G.H. 265 (1997) 320
Warman, J.M., see Piet, J.J. 266 (1997) 70
Warntjes, J.B.M., I. Holleman, G. Meijer and E.J.J. Groenen, Photoluminescence of molecular C_{70} at 1.5 K. On the nature of the lowest excited states 261 (1996) 495
Warren, R.F., see Talukdar, R.K. 262 (1996) 669
Warren, R.W. and B.I. Dunlap, Fractional occupation numbers and density functional energy gradients within the linear combination of Gaussian-type orbitals approach 262 (1996) 384
Warshel, A., Z.T. Chu and W.W. Parson, Two-dimensional free energy surfaces for primary electron transfer in a photosynthetic reaction center 265 (1997) 293
Wasserman, T.A.W., A.A. Arias, T. Müller and P.H. Vaccaro, Degenerate four-wave mixing spectroscopy as a probe of photodissociation dynamics: nascent SH population distributions from the 266 nm photolysis of hydrogen sulfide 262 (1996) 329
Watts, R.O., see Rempe, S.B. 269 (1997) 455
Weaver, M.S., see Lidzey, D.G. 263 (1996) 655
Webb, G.A., see Zheng, G. 266 (1997) 533
Webb, N., see Gadd, G.E. 270 (1997) 108
Weber, P.M., see Ben-Nun, M. 262 (1996) 405
Weeks, D.E., see Calfas, R.S. 263 (1996) 292
Wehrmeister, T., see Baumgarten, M. 267 (1997) 175
Wei, Y., see Plank, R.V. 263 (1996) 33
Weibel, M.A., see Hain, T.D. 262 (1996) 723
Weidinger, A., see Pietzak, B. 265 (1997) 200
Weihe, H. and H.U. Güdel, Kinetic exchange and strong ferromagnetic interactions 261 (1996) 123
Weinkauf, R., see Schiedt, J. 266 (1997) 201
Weitz, E., see House, P.G. 266 (1997) 239
Welge, K.H., see Wrede, E. 265 (1997) 129
Weltner Jr., W., see Li, S. 262 (1996) 298
Weltner Jr., W., see Van Zee, R.J. 266 (1997) 403
Weng, L.-T., see Ding, J. 261 (1996) 92
Weng, Y.-X., H. Xiao, K.-C. Chan and C.-M. Che, Oscillations in a laser-induced chemical reaction: coupling of chemical reactions with an acoustic effect 270 (1997) 315

Werncke, W., M. Pfeiffer, A. Lau, W. Grahn and H.-H. Johannes, Third-order hyperpolarizabilities of a homologous series of meso-nitrogen substituted thiacyanines 266 (1997) 99
Werner, H.-J., see Aoiz, F.J. 262 (1996) 175
Werst, D.W., P. Han and A.D. Trifunac, Trap-to-trap hole transfer studied by radiolysis/EPR. Radical cations in freon and zeolite matrices 269 (1997) 333
Westacott, R.E. and P.M. Rodger, Full-coordinate free-energy minimisation for complex molecular crystals: type I hydrates 262 (1996) 47
Western, C.M., see Cooper, M.J. 267 (1997) 365
Weston, T. and M.S. Child, Spectral consequences of periodic orbit bifurcations of AB_2 stretching vibrational modes 262 (1996) 751
Wheeldon, J.F., see Anderson, A. 263 (1996) 133
Wheeler, M.C., see Seets, D.C. 266 (1997) 431
Wheeler, M.D., A.J. Orr-Ewing, M.N.R. Ashfold and T. Ishiwata, Predissociation lifetimes of the $A^2\Sigma^+$ $v = 1$ state of the SH radical determined by cavity ring-down spectroscopy 268 (1997) 421
Whetten, R.L., see Alvarez, M.M. 266 (1997) 91
White, D., see Šepa, J. 262 (1996) 321
Whittaker, D.M., see Lidzey, D.G. 263 (1996) 655
Wick, M.T., see Ruth, A.A. 266 (1997) 206
Wickleder, C., T. Droz, T. Bürgi and S. Leutwyler, Accurate intermolecular binding energies of 1-naphthol to benzene and cyclohexane 264 (1997) 257
Widmann, E., see Yamazaki, T. 265 (1997) 137
Widmark, P.O., see Engkvist, O. 265 (1997) 19
Wieghardt, K., see Zweygart, W. 261 (1996) 272
Wikrent, P., see Sickafoose, S.M. 263 (1996) 191
Wild, U.P., see Bach, H. 266 (1997) 317
Wild, U.P., see Plakhotnik, T. 262 (1996) 379
Wild, U.P., see Rebane, A. 262 (1996) 155
Wild, U.P., see Walser, D. 270 (1997) 16
Willer, M. and A. Schweiger, Determination of g values by a new electron spin transient nutation experiment: the $g_\perp$ value of titanium-doped sapphire 264 (1997) 1
Willey, K.F., C.L. Brummel and N. Winograd, Photoionization mechanisms for $Cr(CO)_6$ using high intensity laser pulses in the near-IR 267 (1997) 359
Williams, H.L., T. Korona, R. Bukowski, B. Jeziorski and K. Szalewicz, Helium dimer potential from symmetry-adapted perturbation theory 262 (1996) 431
Williams, R.M., J.M. Papanikolas, J. Rathje and S.R. Leone, Quantum-state-resolved 2-level femtosecond rotational coherence spectroscopy: determination of rotational constants at medium and high J in Li_2, a simple diatomic system 261 (1996) 405
Wilson, K.R., see Ben-Nun, M. 262 (1996) 405
Wilson, R.J. and A.J. McCaffery, Velocity selected laser polarization spectroscopy: a powerful and versatile method of obtaining the state-to-state differential cross section 261 (1996) 195
Wilson, W.D., C.M. Schaldach and W.L. Bourcier, Single- and double-layer coupling of Schrödinger and Poisson–Boltzmann equations 267 (1997) 431
Windholz, L., see Li, X. 263 (1996) 463
Windsor, R., see Hamilton, P.A. 264 (1997) 245
Winkler, T., see Mo, Y. 266 (1997) 267
Winkler, T., see Ottinger, Ch. 267 (1997) 294
Winnik, M.A., see Masoumi, Z. 261 (1996) 551
Winograd, N., see Willey, K.F. 267 (1997) 359

Wintterlin, J., see Barth, J.V. 270 (1997) 152
Wirges, W., see Bauer-Gogonea, S. 262 (1996) 663
Wittbrodt, J.M. and H.B. Schlegel, An ab initio study of the thermal decomposition of dichlorosilane 265 (1997) 527
Wittbrodt, J.M. and H.B. Schlegel, An ab initio study of the thermal decomposition of dichlorosilane (Chem. Phys. Letters 265 (1997) 527). Erratum 269 (1997) 391
Witte, G., D. Fuhrmann and Ch. Wöll, Low-energy molecular vibrations investigated by inelastic scattering of He atoms 265 (1997) 347
Wolf, C., see Pietzak, B. 265 (1997) 200
Wolf, H.C., see Gómez, U. 268 (1997) 1
Wolfrum, J., see Brownsword, R.A. 266 (1997) 259
Wolfrum, J., see Müller, R. 262 (1996) 716
Wolfrum, J., see Ko, D.-S. 269 (1997) 54
Wolfrum, J., see Tadday, R. 268 (1997) 117
Wolfsberg, M., see Fritzsche, S. 265 (1997) 253
Wöll, Ch., see Witte, G. 265 (1997) 347
Wolszczak, M., see Szajdzinska-Pietek, E. 270 (1997) 527
Wood, J., see Gadd, G.E. 261 (1996) 221
Woodward, C.A., see Stace, A.J. 267 (1997) 171
Wörgötter, R., V. Grill, Z. Herman, H. Schwarz and T.D. Märk, Low energy reactive and dissociative collisions of the acetone cation $CH_3COCH_3^+$ and its fragment ion CH_3CO^+ with a surface 270 (1997) 333
Wörgötter, R., see Matt, S. 264 (1997) 149
Wöste, L., see Heufelder, J. 269 (1997) 1
Wrachtrup, J., A. Gruber, L. Fleury and C. von Borczyskowski, Magnetic resonance on single nuclei 267 (1997) 179
Wrede, E., L. Schnieder, K.H. Welge, F.J. Aoiz, L. Bañares and V.J. Herrero, High resolution study of the $H + D_2 \rightarrow HD + D$ reaction dynamics at a collision energy of 2.2 eV 265 (1997) 129
Wright, J.C., see Ding, X. 269 (1997) 341
Wright, J.C., see Ding, X. 269 (1997) 72
Wright, J.C., see Lascola, R. 269 (1997) 79
Wright, J.S., D.J. Carpenter, A.B. Alekseyev, H.-P. Liebermann, R. Lingott and R.J. Buenker, Thermodynamically stable diatomic dications: potential curves and radiative lifetimes for $CaCl^{2+}$ including relativistic effects 266 (1997) 391
Wu, G. and X. Ding, The SU(3) algebraic vibrational dynamics of inter-mode couplings: a case study of H_2O, CH_2Br_2 and CD_2Br_2 262 (1996) 421
Wu, G., Global topological approach to highly excited vibration: a case study of H_2O, CH_2Br_2 and CD_2Br_2 270 (1997) 453
Wu, G., Statistical interpretation for the local and normal characters of the SU(3) dynamical system and the symmetry breaking of the equivalent modes 265 (1997) 449
Wu, G., The semiclassical dynamics of electron correlation in the doubly excited coset space: a study of the Hückel model of propenyl and cyclopropenyl systems 264 (1997) 398
Wu, J., see Fang, J. 270 (1997) 145
Wu, M.W. and E.M. Conwell, Transport in α-sexithiophene films 266 (1997) 363
Wu, Z.J., Q.B. Meng and S.Y. Zhang, Ab initio study of C_9 and LaC_9^+ clusters 267 (1997) 271
Wulfov, A.L., Approximate full configuration interaction calculations of total energies, harmonic vibrational frequencies and equilibrium bond distances on F_2, BF, C_2, CN^+ and NO^+ molecules in a DZ + P basis set 263 (1996) 79

Wurzberg, E., see Tserepi, A.D. 265 (1997) 297
Wyatt, R.E., see Ramachandran, B. 270 (1997) 387
Wynne, K., see Haran, G. 261 (1996) 389

Xiao, H., see Weng, Y.-X. 270 (1997) 315
Xiao, M., Local field change of dipole near a surface: a rigorous image theory 270 (1997) 169
Xie, A., see Haran, G. 261 (1996) 389
Xie, M., X.-W. Hou and Z.-Q. Ma, *q*-Deformed harmonic oscillators applied to the vibrational spectrum of methane 262 (1996) 1
Ximei, Q., see Dianxun, W. 262 (1996) 776
Xin, Q.-S. and X.-Y. Zhu, Temperature dependent photodesorption of methyl radical from GaAs: role of the initial state 265 (1997) 259
Xu, C. and D.W. Goodman, Morphology and local electronic structure of metal particles on metal oxide surfaces: a scanning tunneling microscopic and scanning tunneling spectroscopic study 263 (1996) 13
Xu, C. and D.W. Goodman, Structure and geometry of water adsorbed on the MgO(100) surface 265 (1997) 341
Xu, C., see Li, L. 262 (1996) 52
Xu, C.H. and G.E. Scuseria, An O(N) tight-binding study of carbon clusters up to C_{8640}: the geometrical shape of the giant icosahedral fullerenes 262 (1996) 219
Xu, D., see Ding, G. 265 (1997) 392
Xu, G.-Q., see Hrbek, J. 267 (1997) 65
Xu, H.-J., see Tian, H.-J. 263 (1996) 471
Xu, J., see Li, Y. 265 (1997) 361
Xu, W., see Dai, S. 262 (1996) 315
Xue, B., H.-L. Dai and T. Troxler, Structure, electronic relaxation and vibrational predissociation of the electronically excited $SO_2(\tilde{C})$–Ar complex 265 (1997) 154
Xue, G., see Li, F. 264 (1997) 376

Yabushita, S., see Judai, K. 270 (1997) 23
Yacob, A.R., see Mile, B. 263 (1996) 710
Yahioglu, G., see Henari, F.Z. 267 (1997) 229
Yam, V.W.-W., see Kwok, W.M. 262 (1996) 699
Yam, V.W.-W., see Wang, C.-R. 262 (1996) 91
Yamabe, T., see Matsuzaki, Y. 263 (1996) 119
Yamada, S., M. Nakano, I. Shigemoto, S. Kiribayashi and K. Yamaguchi, Intense electron correlation dependence of the first hyperpolarizabilities β of a nitroxide radical and formaldehyde 267 (1997) 445
Yamada, S., M. Nakano, I. Shigemoto, S. Kiribayashi and K. Yamaguchi, Theoretical study of the third-order nonlinear optical susceptibilities for the β-phase crystal of *p*-NPNN 267 (1997) 438
Yamada, S., see Nakano, M. 262 (1996) 66
Yamagishi, H., see Noro, T. 261 (1996) 75
Yamaguchi, H., see Terasaki, A. 262 (1996) 269
Yamaguchi, K., see Kawakami, T. 261 (1996) 129
Yamaguchi, K., see Matsuzaki, Y. 263 (1996) 119
Yamaguchi, K., see Nakano, M. 262 (1996) 66
Yamaguchi, K., see Yamada, S. 267 (1997) 438

Yamaguchi, K., see Yamada, S. 267 (1997) 445
Yamaguchi, K., see Takahashi, H. 264 (1997) 44
Yamaguchi, T., see Ueda, K. 261 (1996) 295
Yamaji, M., T. Tanaka, K. Suto and H. Shizuka, Laser photolysis studies of the formation and decay processes of triplet polyphenyl compounds sensitized by triplet benzophenone 261 (1996) 289
Yamaji, M., see Yoshihara, T. 261 (1996) 431
Yamakage, H., see Teki, Y. 270 (1997) 573
Yamamoto, K., see Ueda, K. 261 (1996) 295
Yamamoto, M., see Ohkita, H. 263 (1996) 602
Yamamoto, N., see Kamiya, N. 265 (1997) 595
Yamanaka, T., Y. Inoue and T. Matsushima, An aligned oxidation of carbon monoxide induced by 193 nm irradiation on platinum(113) 264 (1997) 180
Yamanouchi, K., see Sako, T. 264 (1997) 403
Yamasaki, K., see Tokue, I. 270 (1997) 587
Yamashita, K., see Harima, Y. 262 (1996) 274
Yamashita, K., see Harima, Y. 267 (1997) 481
Yamashita, S., see Oishi, O. 269 (1997) 530
Yamauchi, A., see Bessho, K. 264 (1997) 381
Yamazaki, T., B. Ketzer, E. Widmann, J. Eades, H. Daniel, F.J. Hartmann, M. Hasinoff, R. Pohl, R. Schmidt, T. von Egidy, D. Horváth, M. Kumakura, N. Morita, I. Sugai, Y. Fujita, H.A. Torii, M. Hori, T. Ishikawa, F.E. Maas, H. Tamura and R.S. Hayano, Laser resonance studies of the interactions of metastable antiprotonic helium atomcules $\bar{p}^4He^+$ with surrounding H_2 molecules 265 (1997) 137
Yáñez, M., see González, L. 263 (1996) 407
Yang, C., see Ge, M. 264 (1997) 139
Yang, D., see Vuissoz, P.-A. 264 (1997) 366
Yang, H.-P., see Zhan, J.-P. 264 (1997) 687
Yang, J., see Li, Y. 265 (1997) 361
Yang, Q., see Tian, H.-J. 263 (1996) 471
Yang, S., see Ding, J. 261 (1996) 92
Yang, S., see Gu, G. 270 (1997) 135
Yang, W., see Ding, G. 265 (1997) 392
Yang, W., see York, D.M. 263 (1996) 297
Yarwood, J., see Tassaing, T. 267 (1997) 496
Yasuda, M., see Kobayashi, T. 267 (1997) 472
Yasumatsu, H., see Terasaki, A. 262 (1996) 269
Ye, C., see Zheng, G. 266 (1997) 533
Ye, P.-X., see Tian, H.-J. 263 (1996) 471
Yeh, I.-C., L. Perera and M.L. Berkowitz, Photodetachment spectra of $Cl^-(H_2O)_n$ clusters. Predictions and comparisons 264 (1997) 31
Yekta, A., see Masoumi, Z. 261 (1996) 551
Yeung, P.K.-Y., see Kwok, W.M. 262 (1996) 699
Yi, M. and S. Scheiner, Proton transfer between phenol and ammonia in ground and excited electronic states 262 (1996) 567
Yin, B., see Li, Y. 265 (1997) 361
Ying, L., see Shang, H. 267 (1997) 345
Ylihautala, M., see Koskela, T. 261 (1996) 425
Ynzunza, R., see Chambers, S.A. 267 (1997) 51

Yonekura, N., see Hashimoto, N. 264 (1997) 545
Yonezawa, T., see Vuissoz, P.-A. 264 (1997) 366
Yoo, H.S., see Lee, K. 262 (1996) 610
Yoon, M., see Kim, Y. 264 (1997) 673
York, D.M., T.-S. Lee and W. Yang, Parameterization and efficient implementation of a solvent model for linear-scaling semiempirical quantum mechanical calculations of biological macromolecules 263 (1996) 297
Yoshihara, K., see Saitow, K. 262 (1996) 621
Yoshihara, K., see Inokuchi, Y. 269 (1997) 298
Yoshihara, T., M. Yamaji and H. Shizuka, Laser photolysis studies on hydrogen atom abstraction by triplet benzophenone from hydroxyanilinium ions 261 (1996) 431
Yoshikawa, K., see Noguchi, H. 261 (1996) 527
Yoshimi, K., see Song, M.-B. 263 (1996) 585
Yu, D., see Han, W. 265 (1997) 374
Yu, H.Z., see Zhu, T. 265 (1997) 334
Yu, J., see Zhang, J. 268 (1997) 449
Yuan, Y.N.F., R.A. Eaton and A. Anderson, Far infrared study of carbon disulfide at high pressures 269 (1997) 305
Yuan, Y.N.F., see Eaton, R.A. 269 (1997) 309

Zachariah, M.R., see Berry, R.J. 269 (1997) 107
Zahradník, R., see Nachtigallová, D. 270 (1997) 357
Zaloj, V. and N. Agmon, Electrostatics by Brownian dynamics: solving the Poisson equation near dielectric interfaces 270 (1997) 476
Zambelli, T., see Barth, J.V. 270 (1997) 152
Zander, C., see Müller, R. 262 (1996) 716
Zang, W.-C., see Ding, W. 262 (1996) 259
Zannoni, C., see Berardi, R. 261 (1996) 357
Zannoni, C., see Bacchiocchi, C. 268 (1997) 541
Zare, R.N., see Kandel, S.A. 265 (1997) 121
Zazubovich, S., see Nagirnyi, V. 268 (1997) 280
Zecchina, A., see Lamberti, C. 269 (1997) 500
Zelada, M., see Bosi, L. 267 (1997) 123
Zerner, M.C., see Stavrev, K.K. 263 (1996) 667
Zerza, G., see Sassara, A. 261 (1996) 213
Zetzsch, C., see Jäger, M. 263 (1996) 817
Zgierski, M.Z., see Siebrand, W. 266 (1997) 47
Zhan, C.-G., see Zhao, X. 262 (1996) 643
Zhan, J.-P., W.-Q. Deng, K.-L. Han, H.-P. Yang, G.-Z. He and N.-Q. Lou, Magnetic substate transitions in collisions of Sr(5s5p $^1P_1$) with Ar (Chem. Phys. Letters 260 (1996) 191). Erratum 264 (1997) 687
Zhang, D.H., see Tang, H. 265 (1997) 84
Zhang, H., see Middelhoek, E.R. 267 (1997) 525
Zhang, J. and M. Baumgarten, The stabilities of ground state multiplicities in triradicals and their dependence on configuration and conformation 269 (1997) 187
Zhang, J., S. Huang and J. Yu, Configurational effects in the nonradiative $^5D_2$–$^5D_1$ transition processes of Sm^{2+} in $BaFCl_xBr_{1-x}$ mixed crystals 268 (1997) 449
Zhang, J., see Zhao, L. 263 (1996) 235

Zhang, J.H.Z., see Kouri, D.J. 262 (1996) 519
Zhang, J.Z., see Smith, B.A. 270 (1997) 139
Zhang, K.Q., see Colarusso, P. 269 (1997) 39
Zhang, L., C. Madej, C. Pédrini, B. Moine, C. Dujardin, A. Petrosyan and A.N. Belsky, Elaboration and spectroscopic properties of new dense cerium-doped lutetium based scintillator materials 268 (1997) 408
Zhang, Q., see Wang, D. 266 (1997) 560
Zhang, Q.-E., see Cheng, W.-D. 261 (1996) 66
Zhang, R., see Zhao, L. 263 (1996) 235
Zhang, S., see Gu, G. 270 (1997) 135
Zhang, S.W., see Feng, W.L. 266 (1997) 43
Zhang, S.Y., see Wu, Z.J. 267 (1997) 271
Zhang, X. and C.D. Jonah, Electron solvation in 1-propanol and 2-propanol as a function of temperature 262 (1996) 649
Zhang, X., see Zheng, G. 266 (1997) 533
Zhao, L., J. Zhang, R. Zhang, Y. Li, Y. Chen, R. Cai and Z. Huang, Clustering dynamics of fullerenes in C_{60}/C_{70}-chemically modified poly(N-vinylcarbazole) 263 (1996) 235
Zhao, R., see Ding, G. 265 (1997) 392
Zhao, X., H. Imahori, C.-G. Zhan, Y. Mizutani, Y. Sakata and T. Kitagawa, Ultraviolet resonance Raman spectra and ab initio vibrational analyses of 1,4-benzoquinone: reassignments of the ν_2 and ν_3 bands 262 (1996) 643
Zhao, X., see Shang, H. 267 (1997) 345
Zhao, Z.X., see Guo, L.P. 268 (1997) 26
Zharikov, A.A. and S.F. Fischer, Scaling law for the non-exponential ligand rebinding of CO in myoglobin 263 (1996) 749
Zhdanov, V.P., Comment on: ''Pattern formation by adsorbates with attractive lateral interactions'' 267 (1997) 397
Zheng, G., J. Hu, X. Zhang, L. Shen, C. Ye and G.A. Webb, Quantum chemical calculation and experimental measurement of the ^{13}C chemical shift tensors of vanillin and 3,4-dimethoxybenzaldehyde 266 (1997) 533
Zheng, M., see Silvente, E. 264 (1997) 309
Zheng, Y., see Moler, E.J. 264 (1997) 502
Zhong, W., see Ding, W. 262 (1996) 259
Zhou, Q.-F., see Tian, H.-J. 263 (1996) 471
Zhou, W., see Cheng, C.-F. 263 (1996) 247
Zhu, D., see Li, Y. 265 (1997) 361
Zhu, G. and Y. Hua, Quantitative NMR signal analysis by an iterative quadratic maximum likelihood method 264 (1997) 424
Zhu, L. and C.-F. Ding, Temperature dependence of the near UV absorption spectra and photolysis products of ethyl nitrate 265 (1997) 177
Zhu, T., H.Z. Yu, J. Wang, Y.Q. Wang, S.M. Cai and Z.F. Liu, Two-dimensional surface enhanced Raman mapping of differently prepared gold substrates with an azobenzene self-assembled monolayer 265 (1997) 334
Zhu, X.-Y., see Xin, Q.-S. 265 (1997) 259
Ziegler, J., see Walther, C. 262 (1996) 668
Zikratov, G., D.W. Setser and N. Sadeghi, Radiative lifetimes, vibrational band strengths, relaxation mechanisms, and electronic transfer rate constants for the perturbed CO($a'\,^3\Sigma^+$, $v' = 31$ and 35) levels 265 (1997) 585

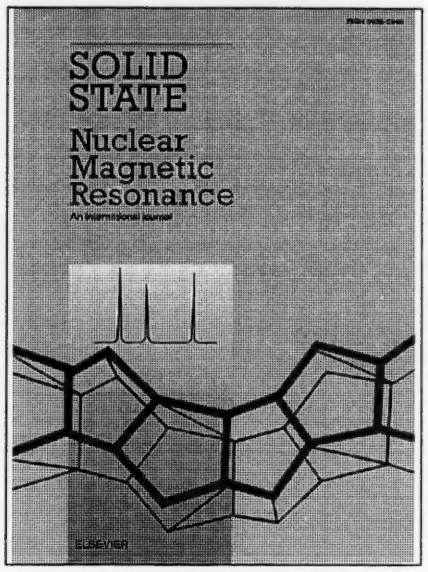
Zinth, W., see Hamm, P. 263 (1996) 613
Zinth, W., see Hamm, P. 268 (1997) 180
Ziurys, L.M., see Allen, M.D. 270 (1997) 517
Zolotov, B., A. Gan, B.D. Fainberg and D. Huppert, Resonance heterodyne optical Kerr spectroscopy of solvation dynamics in water and D_2O 265 (1997) 418
Zon, B.A., Born–Oppenheimer approximation for molecules in a strong light field 262 (1996) 744
Zorić, I., see Åkerlund, C. 270 (1997) 157
Zoriniants, G.E., see Frankevich, E.L. 261 (1996) 545
Zoriniants, G.E., see Tarasov, V.V. 267 (1997) 58
Zschokke-Gränacher, I., see Bopp, M.A. 263 (1996) 721
Zuo, J., see Li, L. 262 (1996) 52
Zurek, M., see Hamm, P. 263 (1996) 613
Zurek, M., see Hamm, P. 268 (1997) 180
Zvejnieks, G.J., see Kalnin, Yu.R.H. 270 (1997) 229
Zweygart, W., R. Bittl, K. Wieghardt and W. Lubitz, EPR and ^{55}Mn cw-ENDOR study of an antiferrogmagnetically coupled dinuclear manganese ($Mn^{III}Mn^{IV}$) complex 261 (1996) 272
Zwier, T.S., see Pribble, R.N. 262 (1996) 627
Zyss, J., see Bauer-Gogonea, S. 262 (1996) 663

Send for a Free Sample Copy!

Solid State Nuclear Magnetic Resonance

An International Journal

- *"Papers of uniformly excellent quality..."* **(Nature, October 1993)**
- **Only truly international journal dealing with all aspects of solid state NMR**
- **Short communications section: rapid publication of research results when fast publication is warranted**
- **Free contents alerting service via e-mail**



Editor-in-Chief:
J. Klinowski, *University of Cambridge, Department of Chemistry, Lensfield Road, Cambridge CB2 1EW, UK. Fax: (44-1223) 336362, E-mail: jk18@cus.cam.ac.uk*

AIMS AND SCOPE:

The journal *Solid State Nuclear Magnetic Resonance* publishes original manuscripts of high scientific quality dealing with all experimental and theoretical aspects of solid state NMR. Typical areas for applications include: solid state chemistry, materials science; surface chemistry, catalysis; polymer science and characterization; geology, mineralogy; biochemistry, biology, medicine; physics.

For:
Academic and Industrial Researchers engaged in the development of new NMR techniques and their application to structural analysis.

Solid State Nuclear Magnetic Resonance
http://www.elsevier.nl/locate/solmag

❑ Please send me a **FREE Sample Copy** including instructions to authors

Name: ..... Initials: .....
Position: ..... Title: .....
Institute/Company: .....
Department: .....
Address: .....
Post/Zip Code: ..... City: .....
Country: ..... Tel: .....
Fax: ..... E-mail address: .....

ELSEVIER SCIENCE

New York
Tel: (+1) 212-633-3730
[Toll Free number for North American customers: 1-888-4ES-INFO (437-4636)]
Fax: (+1) 212-633-3680
E-mail: usinfo-f@elsevier.com

Amsterdam
Tel: (+31) 20-485-3757
Fax: (+31) 20-485-3432
E-mail: nlinfo-f@elsevier.nl

Tokyo
Tel: (+81) 3-5561-5033
Fax: (+81) 3-5561-5047
E-mail: info@elsevier.co.jp

Singapore
Tel: (+65) 434-3727
Fax: (+65) 337-2230
E-mail: asiainfo@elsevier.com.sg

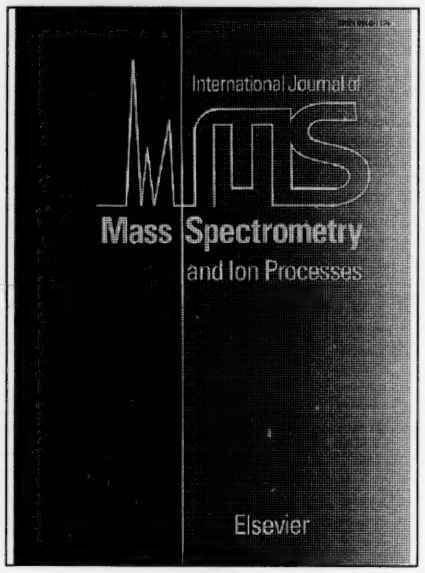
Please quote the following code with all requests: MD7

12/97

Send for a Free Sample Copy!

International Journal of Mass Spectrometry and Ion Processes

- **Includes Letters for fast publication (about 2 months) of "hot" results**
- **THE publication outlet for *new* developments in the field**
- **Features two awards for the Best Student Paper annually**
- **Elsevier mass spectrometry online service http://www.elsevier.nl/locate/maspec-online**
- **Free contents alerting service via e-mail**



Editors:

M.T. Bowers, *University of California, Department of Chemistry, Santa Barbara, CA 93106, USA.*
Fax: (1-805) 893-8703/4120, E-mail: bowers@sbmm1.ucsb.edu,
H. Schwarz, *Technical University, Department of Chemistry, Strasse des 17. Juni 135, D-10623 Berlin, Germany.*
Fax: (49-30) 3142-1102, E-mail: schw0531@zrzsp5.chem.tu-berlin.de
J.F.J. Todd, *University Chemical Laboratory, University of Kent, Canterbury, Kent CT2 7NH, UK.*
Fax: (44-1227) 475475, E-mail: j.f.j.todd@ukc.ac.uk

AIMS AND SCOPE:

The journal contains papers which consider fundamental aspects of mass spectrometry and ion processes and the study of the application of mass spectrometric techniques to specific problems in chemistry and physics. The *International Journal of Mass Spectrometry and Ion Processes* is the leading journal for publishing new developments in the field.

For:
All Mass Spectrometrists and others interested in the chemistry and physics of charged particles.

International Journal of Mass Spectrometry and Ion Processes
http://www.elsevier.nl/locate/ijmsip

❑ Please send me a **FREE Sample Copy** including instructions to authors

Name: ..... Initials: .....
Position: ..... Title: .....
Institute/Company: .....
Department: .....
Address: .....
Post/Zip Code: ..... City: .....
Country: ..... Tel: .....
Fax: ..... E-mail address: .....

ELSEVIER SCIENCE

New York
Tel: (+1) 212-633-3730
[Toll Free number for North American customers: 1-888-4ES-INFO (437-4636)]
Fax: (+1) 212-633-3680
E-mail: usinfo-f@elsevier.com

Amsterdam
Tel: (+31) 20-485-3757
Fax: (+31) 20-485-3432
E-mail: nlinfo-f@elsevier.nl

Tokyo
Tel: (+81) 3-5561-5033
Fax: (+81) 3-5561-5047
E-mail: info@elsevier.co.jp

Singapore
Tel: (+65) 434-3727
Fax: (+65) 337-2230
E-mail: asiainfo@elsevier.com.sg

Please quote the following code with all requests: MD7

12/97

Orders, claims, and product enquiries: please contact the Customer Support Department at the Regional Sales Office nearest to you:

New York
Elsevier Science
P.O. Box 945
New York, NY 10159-0945
USA
Tel. (+1)212-633-3730
[Toll free number for North American customers: 1-888-4ES-INFO (437-4636)]
Fax (+1)212-633-3680
e-mail: usinfo-f@elsevier.com

Amsterdam
Elsevier Science
P.O. Box 211
1000 AE Amsterdam
The Netherlands
Tel. (+31)20-4853757
Fax (+31)20-4853432
e-mail: nlinfo-f@elsevier

Tokyo
Elsevier Science
9-15 Higashi-Azabu 1-chome
Minato-ku, Tokyo 106
Japan
Tel. (+81)3-5561-5033
Fax (+81)3-5561-5047
e-mail: kyf04035@niftyserve.or.jp

Singapore
Elsevier Science
No. 1 Temasek Avenue
#17-01 Millenia Tower
Singapore 039192
Tel. (+65)434-3727
Fax (+65)337-2230
e-mail: asiainfo@elsevier.com.sg

Advertising information: Advertising orders and enquiries may be sent to: **International:** Elsevier Science, Advertising Department, The Boulevard, Langford Lane, Kidlington, Oxford OX5 1GB, UK, Tel. (+44)(0)1865 843565, Fax (+44)(0)1865 843976. **USA and Canada:** Weston Media Associates, Daniel Lipner, P.O. Box 1110, Greens Farms, CT 06436-1110, USA, Tel. (+1)(203)261-2500, Fax (+1)(203)261-0101. **Japan:** Elsevier Science Japan, Marketing Services, 1-9-15 Higashi-Azabu, Minato-ku, Tokyo 106, Japan, Tel. (+81)3-5561-5033, Fax (+81)3-5561-5047.

Electronic manuscripts: Electronic manuscripts have the advantage that there is no need for the rekeying of text, thereby avoiding the possibility of introducing errors and resulting in reliable and fast publication.

Your disk plus three, final and exactly matching printed versions should be submitted together. Double density (DD) or high density (HD) diskettes ($3^1/2$ or $5^1/4$ inch) are acceptable. It is important that the file saved is in the native format of the wordprocessor program used. Label the disk with the name of the computer and wordprocessing package used, your name, and the name of the file on the disk. Further information may be obtained from the Publisher.

Authors in Japan please note: Upon request, Elsevier Science Japan will provide authors with a list of people who can check and improve the English of their paper (*before submission*). Please contact our Tokyo office: Elsevier Science Japan, 1-9-15 Higashi-Azabu, Minato-ku, Tokyo 106; Tel. (03)-5561-5032; Fax (03)-5561-5045.

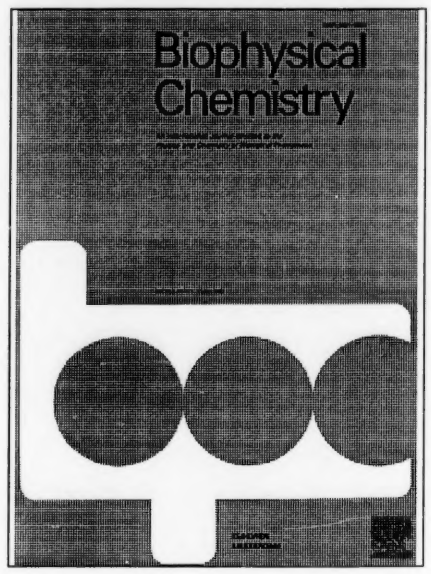
Chemical Physics Letters has no page charges.

For a full and complete Instructions to Authors, please refer to *Chemical Physics Letters,* Vol. 270, No. 5,6, pp. 609–610. The instructions can also be found on the World Wide Web: access under http://www.elsevier.nl or http://www.elsevier.com.

♾ The paper used in this publication meets the requirements of ANSI/NISO Z39.48-1992 (Permanence of Paper)

Send for a Free Sample Copy!

Biophysical Chemistry



An International Journal devoted to the Physics and Chemistry of Biological Phenomena

- **Only journal especially devoted to research on borderline of chemistry, biology and physics**
- **Letters section: publication time of about 3 months**
- **Free colour pictures and other supplementary material on www**
- **Free contents alerting service via e-mail**

Principal Editor:
A. Watts, *University of Oxford, Department of Biochemistry, South Parks Road, Oxford OX1 3QU, UK.*
Fax: (44-1865) 275234/59,
E-mail: awatts@bioch.ox.ac.uk

AIMS AND SCOPE:
The journal publishes original letters and papers, mini-reviews, reports from meetings and special issues describing research on biological phenomena in terms of the principles and methods of physics and chemistry. It is receptive to articles which deal with biological molecules and systems, and to papers which treat systems serving as models for these. Treatments, phenomenological as well as molecular, of the interactions, structure and biological functions of individual biological macromolecules and of supramolecular structures, are also within the journal's remit.

For:
Biophysicists, Physical Chemists, Chemical Physicists and Biochemists.

Biophysical Chemistry
http://www.elsevier.nl/locate/bpc

❑ Please send me a **FREE Sample Copy** including instructions to authors

Name: ..... Initials: .....
Position: ..... Title: .....
Institute/Company: .....
Department: .....
Address: .....
Post/Zip Code: ..... City: .....
Country: ..... Tel: .....
Fax: ..... E-mail address: .....

ELSEVIER SCIENCE

New York
Tel: (+1) 212-633-3730
[Toll Free number for North American customers: 1-888-4ES-INFO (437-4636)]
Fax: (+1) 212-633-3680
E-mail: usinfo-f@elsevier.com

Amsterdam
Tel: (+31) 20-485-3757
Fax: (+31) 20-485-3432
E-mail: nlinfo-f@elsevier.nl

Tokyo
Tel: (+81) 3-5561-5033
Fax: (+81) 3-5561-5047
E-mail: info@elsevier.co.jp

Singapore
Tel: (+65) 434-3727
Fax: (+65) 337-2230
E-mail: asiainfo@elsevier.com.sg

Please quote the following code with all requests: MD7

12/97

0009-2614(199706)261/270;1-P